CHEMICAL ENGINEERING DESIGN

PRINCIPLES, PRACTICE AND ECONOMICS OF PLANT AND PROCESS DESIGN

THIRD EDITION

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Ray Sinnott

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Preface to the Third Edition

This book was originally written by Ray Sinnott as Volume 6 of the "Chemical Engineering" series edited by Coulson and Richardson. It was intended to be a standalone design textbook for undergraduate design projects that would supplement the other volumes in the Coulson and Richardson series. In 2008 we published the first edition of *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design* as an adaptation of Coulson and Richardson Volume 6 for the North American market. Some older sections of the book were updated, and references to laws, codes, and standards were changed to an American rather than British basis; however, the general layout and philosophy of the book remained unaltered.

The first edition of this book was widely adopted, and I received a great deal of valuable feedback from colleagues on both the strengths and weaknesses of the text in the context of a typical North American undergraduate curriculum. The experiences and frustrations of my students at Northwestern University and comments from coworkers at Honeywell UOP also helped suggest areas where the book could be improved. The second edition rearranged the material substantially to make the book more valuable to students and industrial practitioners by incorporating new material to address obvious gaps, while eliminating some material that was dated or repetitive of foundation classes. The book was divided into two parts. Part I: Process Design covers the topics that are typically taught in a lecture class on process design and economics. The broad themes of Part I are flowsheet development, economic analysis, safety and environmental impact, and optimization. Part II: Plant Design contains chapters on equipment design and selection that can be used as supplements to a lecture course. These chapters contain step-by-step methods for designing most unit operations, together with many worked examples, and should become essential references for students when they begin working through their design projects or face design problems early in their industrial career. The third edition retains the same format and has been updated throughout to reflect legislative changes, the most recent codes and standards, and updated information on process and equipment costs.

Chemical engineers work in a very diverse set of industries, and many of these industries have their own design conventions and specialized equipment. I have attempted to include examples and problems from a broad range of process industries, but where space or my lack of expertise in the subject has limited coverage of a particular topic, references to specialized texts are provided.

This book draws on Ray Sinnott's and my experience of the industrial practice of process design, as well as our experience teaching design at the University of Wales Swansea, University of Manchester, Northwestern University, and National University of Singapore. Since the book is intended to be used in practice and not just as a textbook, our aim has been to describe the tools and methods that are most widely used in industrial process design. We have deliberately avoided describing idealized conceptual methods that have not yet gained wide currency in industry. The reader can find good descriptions of these methods in the research literature and in more academic textbooks.

Standards and codes of practice are an essential part of engineering, and the relevant North American standards are cited. The codes and practices covered by these standards will be applicable to other countries. They will be covered by equivalent national standards in most developed countries, and in some cases the relevant British, European, or international standards have also been cited. Brief summaries of important U.S. and Canadian safety and environmental legislation have been given in the relevant chapters. The design engineer should always refer to the original source references of laws, standards, and codes of practice, as they are updated frequently.

Most industrial process design is carried out using commercial design software. Extensive reference has been made to commercial process and equipment design software throughout the book. Many of the commercial software vendors provide licenses of their software for educational purposes at nominal fees. I strongly believe that students should be introduced to commercial software at as early a stage in their education as possible. The use of academic design and costing software should be discouraged. Academic programs usually lack the quality control and support required by industry, and the student is unlikely to use such software after graduation. All computer-aided design

tools must be used with some discretion and engineering judgment on the part of the designer. This judgment mainly comes with experience, but I have tried to provide helpful tips on how to best use computer tools.

Ray wrote in the preface to the first edition of his book: "*The art and practice of design cannot be learned from books. The intuition and judgment necessary to apply theory to practice will come only from practical experience.*" As with all our previous editions, I hope that this latest edition will make it easier for readers to begin acquiring that experience.

Gavin Towler

How To Use This Book

This book has been written primarily for students on undergraduate courses in chemical engineering and has particular relevance to their senior design projects. It should also be of interest to new graduates working in industry who find they need to broaden their knowledge of unit operations and design. Some of the earlier chapters of the book can also be used in introductory chemical engineering classes and by other disciplines in the chemical and process industries.

PART I: PROCESS DESIGN

Part I has been conceived as an introductory course in process design. The material can be covered in 20 to 30 lecture hours, and presentation slides are available to qualified instructors in the supplementary material available at www.elsevier.com/books-and-journals/book-companion/9780128211793. Chapter 1 is a general overview of process design and contains an introductory section on product design. Chapter 2, Chapter 3, Chapter 4, Chapter 5, and Chapter 6 address the development of a process flowsheet from initial concept to the point where the designer is ready to begin estimating capital costs. Chapter 2 covers the selection of major unit operations and also addresses design for revamps and modification of conventional flowsheets. Chapter 3 introduces utility systems and discusses process energy recovery and heat integration. Chapter 4 provides an introduction to process simulation and shows the reader how to complete process material and energy balances. Chapter 5 covers those elements of process control that must be understood to complete a process flow diagram and identify where pumps and compressors are needed in the flowsheet. The selection of materials of construction can have a significant effect on plant costs, and this topic is addressed in Chapter 6. The elements of process economic analysis are introduced in Chapter 7, Chapter 8, and Chapter 9. Capital cost estimation is covered in Chapter 7. Operating costs, revenues, and price forecasting are treated in Chapter 8. Chapter 9 concludes the economics section of the book with a brief introduction to corporate finance, a description of economic analysis methods, and a discussion on project selection criteria used in industry. Chapter 10 examines the role of safety considerations in design and introduces the methods used for process hazard analysis. Chapter 11 addresses site design and environmental impact. Part I concludes with a discussion of optimization methods in Chapter 12.

PART II: PLANT DESIGN

Part II contains a more detailed treatment of design methods for common unit operations. Chapter 13 provides an overview of equipment design and is also a guide to the following chapters. Chapter 14 discusses the design of pressure vessels and provides the necessary background for the reader to be able to design reactors, separators, distillation columns, and other operations that must be designed under pressure vessel codes. Chapter 15 covers the design of mixers and reactors, with an emphasis on the practical mechanical layout of reactors. Chapter 16 and Chapter 17 address fluid phase separations. Multistage column separations (distillation, absorption, stripping, and extraction) are described in Chapter 17, while other separation processes, such as adsorption, membrane separation, decanting, crystallization, precipitation, ion exchange, and chromatography, are covered in Chapter 16. Chapter 18 examines the properties of granular materials and introduces the processes used for storing, conveying, mixing, separating, heating, drying, and altering the particle size distribution of solids. Chapter 19 covers all aspects of the design of heat-transfer equipment, including plate exchangers, air coolers, fired heaters, and direct heat transfer to vessels, as well as design of shell and tube heat exchangers, boilers, and condensers. Chapter 20 addresses the design of plant hydraulics and covers design and selection of pumps, compressors, piping systems, and control valves. The material in Part II can be used to provide supplementary lectures in a design class or as a supplement to foundation

courses in chemical engineering. The chapters have also been written to serve as a guide to selection and design, with extensive worked examples, so that students can dip into individual chapters as they face specific design problems when working on a senior year design project.

SUPPLEMENTARY MATERIAL

Many of the calculations described in the book can be performed using spreadsheets. Templates of spreadsheet calculations and equipment specification sheets are available in Microsoft Excel format online and can be downloaded from www.elsevier.com/books-and-journals/book-companion/9780128211793. An extensive set of design problems are included in the Appendices, which are also available at the same website.

Additional supplementary material, including Microsoft PowerPoint presentations to support most of the chapters and a full solutions manual, are available only to instructors, by registering at the Instructor section on https://educate.elsevier.com/9780128211793.

Acknowledgments

As stated in the preface, after launching the first edition of this book I received a great deal of very valuable feedback from students and colleagues. I have tried to make good use of this feedback in the second and third editions. Particular thanks are due to John Baldwin, Michael Caracotsios, Elizabeth Carter, Dan Crowl, Mario Eden, Mahmoud El-Halwagi, Igor Kourkine, Harold Kung, Justin Notestein, A.V. Purushothaman, Matthew Realff, Tony Rogers, Warren Seider, Farzin Shemirani, Bill Wilcox, and Dave Wegerer, all of whose suggestions I have gratefully incorporated. Many further improvements were suggested during the review phase, and I would like to thank Mark James, Barry Johnston, Ken Joung, Yoshiaki Kawajiri, Peg Stine, Ross Taylor, and Andy Zarchy for their thoughtful reviews and input. Rajeev Gautam and Ben Christolini allowed me to pursue this project and make use of Honeywell UOPs extensive technical resources. As always, many colleagues at Honeywell UOP, AIChE, and CACHE and students and colleagues at Northwestern and National University of Singapore have shared their experience and given me new insights into chemical engineering design and education.

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The supplementary material contains images of processes and equipment from many sources. I would like to thank the following companies for permission to use these images: Alfa-Laval, ANSYS, Aspen Technology, Bete Nozzle, Bos-Hatten Inc., Chemineer, Dresser, Dresser-Rand, Enardo Inc., Honeywell, Komax Inc., Riggins Company, Tyco Flow Control Inc., United Valve Inc., Honeywell UOP LLC, and The Valve Manufacturers Association.

Stephen Merken led the Elsevier team in developing this book and provided much useful editorial guidance. I would also like to thank Beth LoGiudice and Kamatchi Madhavan for their excellent work in managing all the stages of production and printing.

The biggest debt that I must acknowledge is to my coauthor, Ray Sinnott. Although Ray was not involved in writing this edition, it is built on the foundation of his earlier work, and his words can be found in every chapter. I hope I have remained true to Rays philosophy of design and have preserved the strengths of his book. It was necessary for me to remove some older material to make space for new sections in the book, and I hope that Ray will forgive these changes. Needless to say, I am entirely responsible for any deficiencies or errors that have been introduced.

My regular job at Honeywell UOP keeps me very busy, and I worked on this book in the evenings and on the weekends, so it would not have been possible without the love and support of my wife, Xiaona, and our children Miranda, Jimmy, Andrew and Michael.

Gavin P. Towler
Inverness, Illinois

CHAPTER

1

Introduction to design

KEY LEARNING OBJECTIVES

- How design projects are carried out and documented in industry, including the formats used for design reports
- Why engineers in industry use codes and standards in design
- Why it is necessary to build margins into a design
- Methods used by product design engineers to translate customer needs into product specifications

1.1 Introduction

This chapter is an introduction to the nature and methodology of the design process and its application to the design of chemical products and manufacturing processes.

1.2 Nature of design

This section is a general discussion of the design process. The subject of this book is chemical engineering design, but the methodology described in this section applies equally to other branches of engineering.

Chemical engineering has consistently been one of the highest-paid engineering professions. There is a demand for chemical engineers in many sectors of industry, including the traditional process industries: chemicals, polymers, fuels, foods, pharmaceuticals, and paper, as well as other sectors such as electronic materials and devices, consumer products, mining and metals extraction, biomedical implants, and power generation.

The reason that companies in such a diverse range of industries value chemical engineers so highly is the following:

> Starting from a vaguely defined problem statement such as a customer need or a set of experimental results, chemical engineers can develop an understanding of the important underlying physical science relevant to the problem and use this understanding to create a plan of action and set of detailed specifications, which if implemented, will lead to a predicted financial outcome.

The creation of plans and specifications and the prediction of the financial outcome if the plans are implemented is the activity of chemical engineering design.

Design is a creative activity, and as such can be one of the most rewarding and satisfying activities undertaken by an engineer. The design does not exist at the start of the project. The designer begins with a specific objective or

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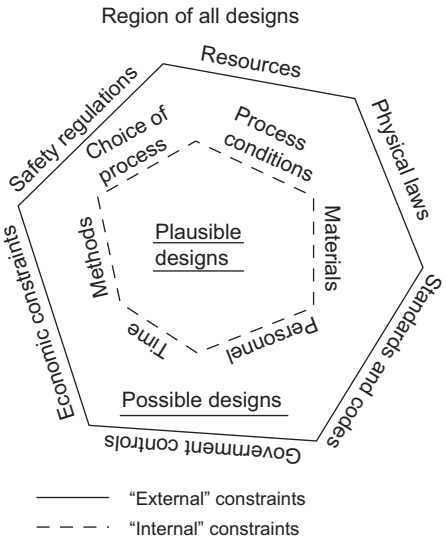


FIG. 1.1 Design constraints.

customer need in mind, and by developing and evaluating possible designs, arrives at the best way of achieving that objective, be it a better chair, a new bridge, or for the chemical engineer, a new chemical product or production process.

When considering possible ways of achieving the objective the designer will be constrained by many factors, which will narrow down the number of possible designs. There will rarely be just one possible solution to the problem, just one design. Several alternative ways of meeting the objective will normally be possible, even several best designs, depending on the nature of the constraints.

These constraints on the possible solutions to a problem in design arise in many ways. Some constraints will be fixed and invariable, such as those that arise from physical laws, government regulations, and engineering standards. Others will be less rigid and can be relaxed by the designer as part of the general strategy for seeking the best design. The constraints that are outside the designer's influence can be termed *the external constraints*. These set the outer boundary of possible designs, as shown in Fig. 1.1. Within this boundary there will be a number of plausible designs bounded by the other constraints, the internal constraints, over which the designer has some control; this can include choice of process, choice of process conditions, materials, and equipment.

Economic considerations are obviously a major constraint on any engineering design: plants must make a profit. Process costing and economics are discussed in Chapters 7, 8, and 9.

Time will also be a constraint. The time available for completion of a design will usually limit the number of alternative designs that can be considered.

The stages in the development of a design, from the initial identification of the objective to the final design, are shown diagrammatically in Fig. 1.2. Each stage is discussed in the following sections.

Fig. 1.2 shows design as an iterative procedure. As the design develops, the designer will become aware of more possibilities and more constraints and will be constantly seeking new data and evaluating possible design solutions.

1.2.1 The design objective (the need)

All design starts with a perceived need. In the design of a chemical product or process, the need is the public need for the product, creating a commercial opportunity, as foreseen by the sales and marketing organization. Within this overall objective the designer will recognize subobjectives: the requirements of the various units that make up the overall process.

Before starting work, the designer should obtain as complete, and as unambiguous, a statement of the requirements as possible. If the requirement (need) arises from outside the design group, from a customer or from another department, then the designer will have to elucidate the real requirements through discussion. It is important to distinguish between the needs that are "must-haves" and those that are "should-haves." The "should-haves" are

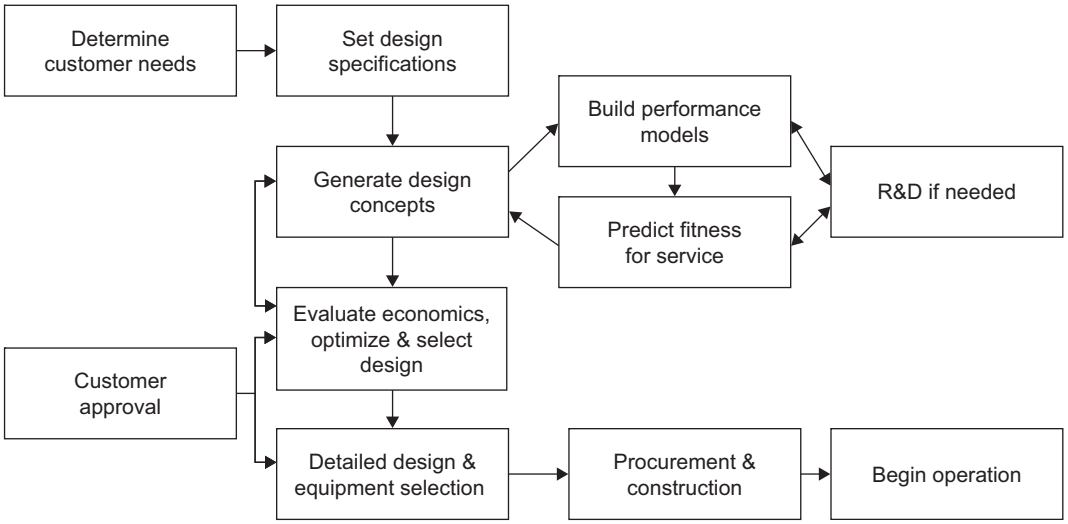


FIG. 1.2 The design process.

those parts of the initial specification that may be thought desirable but that can be relaxed if necessary as the design develops. For example, a particular product specification may be considered desirable by the sales department but may be difficult and costly to obtain, and some relaxation of the specification may be possible, producing a saleable but cheaper product. Whenever possible, the designer should always question the design requirements (the project and equipment specifications) and keep them under review as the design progresses. It is important for the design engineer to work closely with the sales or marketing department or with the customer directly to have as clear as possible an understanding of the customer's needs.

When writing specifications for others, such as for the mechanical design or purchase of a piece of equipment, the design engineer should be aware of the restrictions (constraints) that are being placed on other designers. A well-thought-out, comprehensive specification of the requirements for a piece of equipment defines the external constraints within which the other designers must work.

1.2.2 Setting the design basis

The most important step in starting a process design is translating the customer need into a design basis. The design basis is a more precise statement of the problem that is to be solved. It will normally include the production rate and purity specifications of the main product, together with information on constraints that will influence the design, such as:

1. The system of units to be used.
2. The national, local, or company design codes that must be followed.
3. Details of raw materials that are available.
4. Information on potential sites where the plant might be located, including climate data, seismic conditions and infrastructure availability. Site design is discussed in detail in Chapter 11.
5. Information on the conditions, availability, and price of utility services such as fuel gas, steam, cooling water, process air, process water, and electricity that will be needed to run the process.

The design basis must be clearly defined before design can begin. If the design is carried out for a client, then the design basis should be reviewed with the client at the start of the project. Most companies use standard forms or questionnaires to capture design basis information. An example template is given in Appendix G and can be downloaded in Microsoft Excel format from the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

1.2.3 Generation of possible design concepts

The creative part of the design process is the generation of possible solutions to the problem for analysis, evaluation, and selection. In this activity most designers largely rely on previous experience, their own and that of others. It is doubtful if any design is entirely novel. The antecedence of most designs can usually be easily traced. The first motor cars were clearly horse-drawn carriages without the horse, and the development of the design of the modern car can be traced step by step from these early prototypes. In the chemical industry, modern distillation processes have developed from the ancient stills used for rectification of spirits, and the packed columns used for gas absorption have developed from primitive, brushwood-packed towers. So, it is not often that a process designer is faced with the task of producing a design for a completely novel process or piece of equipment.

Experienced engineers usually prefer the tried and tested methods rather than possibly more exciting but untried novel designs. The work that is required to develop new processes, and the cost, are usually underestimated. Commercialization of new technology is difficult and expensive, and few companies are willing to make multimillion-dollar investments in technology that is not well proven (a phenomenon known in industry as *"me third" syndrome*). Progress is made more surely in small steps; however, when innovation is wanted, previous experience, through prejudice, can inhibit the generation and acceptance of new ideas (known as *"not invented here" syndrome*).

The amount of work, and the way it is tackled, will depend on the degree of novelty in a design project. Development of new processes inevitably requires much more interaction with researchers and collection of data from laboratories and pilot plants.

Chemical engineering projects can be divided into three types, depending on the novelty involved:

1. Modifications and additions to an existing plant, usually carried out by the plant design group. Projects of this type represent about half of all the design activity in industry.
2. New production capacity to meet growing sales demand and the sale of established processes by contractors. Repetition of existing designs, with only minor design changes, including designs of vendor's or competitor's processes carried out to understand whether they have a compellingly better cost of production. Projects of this type account for about 45% of industrial design activity.
3. New processes developed from laboratory research, through pilot plant to a commercial process. Even here, most of the unit operations and process equipment will use established designs. This type of project accounts for less than 5% of design activity in industry.

The majority of process designs are based on designs that previously existed. The design engineer very rarely sits down with a blank sheet of paper to create a new design from scratch, an activity sometimes referred to as *"process synthesis."* Even in industries such as pharmaceuticals, where research and new product development are critically important, the types of processes used are often based on previous designs for similar products, so as to make use of well-understood equipment and smooth the process of obtaining regulatory approval for the new plant.

The first step in devising a new process design will be to sketch out a rough block diagram showing the main stages in the process and to list the primary function (objective) and the major constraints for each stage. Experience should then indicate what types of unit operations and equipment should be considered. The steps involved in determining the sequence of unit operations that constitutes a process flowsheet are described in Chapter 2.

The generation of ideas for possible solutions to a design problem cannot be separated from the selection stage of the design process; some ideas will be rejected as impractical as soon as they are conceived.

1.2.4 Fitness testing

When design alternatives are suggested, they must be tested for fitness for purpose. In other words, the design engineer must determine how well each design concept meets the identified need. In the design of chemical plants, it is usually prohibitively expensive to build several designs to find out which one works best. Instead, the design engineer builds a mathematical model of the process, usually in the form of computer simulations of the process, reactors, and other key equipment. In some cases, the performance model may include a pilot plant or other facility for predicting plant performance and collecting the necessary design data. In other cases, the design data can be collected from an existing full-scale facility or can be found in the chemical engineering literature.

The design engineer must assemble all of the information needed to model the process so as to predict its performance against the identified objectives. For process design, this will include information on possible processes, equipment performance, and physical property data. Sources of process information are reviewed in Chapter 2.

Many design organizations will prepare a basic data manual containing all the process "know-how" on which the design is to be based. Most organizations will have design manuals covering preferred methods and data for the more frequently used design procedures. The national standards are also sources of design methods and data. They are also design constraints, as new plants must be designed in accordance with national standards and regulations. If the necessary design data or models do not exist, then research and development work is needed to collect the data and build new models.

Once the data have been collected and a working model of the process has been established, the design engineer can begin to determine equipment sizes and costs. At this stage it will become obvious that some designs are uneconomical and they can be rejected without further analysis. It is important to make sure that all of the designs that are considered are fit for the service (i.e., meet the customer's "must-have" requirements). In most chemical engineering design problems this comes down to producing products that meet the required specifications. A design that does not meet the customer's objective can usually be modified until it does so, but this always adds extra costs.

1.2.5 Economic evaluation, optimization, and selection

Once the designer has identified a few candidate designs that meet the customer objective, then the process of design selection can begin. The primary criterion for design selection is usually economic performance, although factors such as safety and environmental impact may also play a strong role. The economic evaluation usually entails analyzing the capital and operating costs of the process to determine the return on investment, as described in Chapters 7, 8, and 9.

The economic analysis of the product or process can also be used to optimize the design. Every design will have several possible variants that make economic sense under certain conditions. For example, the extent of process heat recovery is a trade-off between the cost of energy and the cost of heat exchangers (usually expressed as a cost of heat exchange area). In regions where energy costs are high, designs that use a lot of heat exchange surface to maximize recovery of waste heat for reuse in the process will be attractive. In regions where energy costs are low, it may be more economical to burn more fuel and reduce the capital cost of the plant. Techniques for energy recovery are described in Chapter 3. The mathematical techniques that have been developed to assist in the optimization of plant design and operation are discussed briefly in Chapter 12.

When all of the candidate designs have been optimized, the best design can be selected. Very often, the design engineer will find that several designs have very close economic performance, in which case the safest design or that which has the best commercial track record will be chosen. At the selection stage an experienced engineer will also look carefully at the candidate designs to make sure that they are safe, operable, and reliable and to ensure that no significant costs have been overlooked.

1.2.6 Detailed design and equipment selection

After the process or product concept has been selected, the project moves on to detailed design. Here the detailed specifications of equipment such as vessels, exchangers, pumps, and instruments are determined. The design engineer may work with other engineering disciplines, such as civil engineers for site preparation, mechanical engineers for design of vessels and structures, and electrical engineers for instrumentation and control.

Many companies engage specialist engineering, procurement, and construction (EPC) companies, commonly known as *contractors*, at the detailed design stage. The EPC companies maintain large design staffs who can quickly and competently execute projects at relatively low cost.

During the detailed design stage there may still be some changes to the design, and there will certainly be ongoing optimization as a better idea of the project cost structure is developed. The detailed design decisions tend to focus mainly on equipment selection, though, rather than on changes to the flowsheet. For example, the design engineer may need to decide whether to use a U-tube or a floating-head exchanger, as discussed in Chapter 19, or whether to use trays or packing for a distillation column, as described in Chapter 17.

1.2.7 Procurement, construction, and operation

When the details of the design have been finalized, the equipment can be purchased and the plant can be built. Procurement and construction are usually carried out by an EPC firm unless the project is very small. Because they work on many different projects each year, the EPC firms are able to place bulk orders for items such as piping, wire, valves, etc., and can use their purchasing power to get discounts on most equipment. The EPC companies also have a great deal of experience in field construction, inspection, testing, and equipment installation. They can therefore normally contract to build a plant for a client cheaper (and usually also quicker) than the client could build it on their own.

Finally, once the plant is built and readied for start-up, it can begin operation. The design engineer will often then be called upon to help resolve any start-up issues and teething problems with the new plant.

1.3 The organization of a chemical engineering project

The design work required in the engineering of a chemical manufacturing process can be divided into two broad phases.

Phase 1: Process design, which covers the steps from the initial selection of the process to be used through to the issuing of the process flowsheets and includes the selection, specification, and chemical engineering design of equipment. In a typical organization, this phase is the responsibility of the process design group, and the work is mainly done by chemical engineers. The process design group may also be responsible for the preparation of the piping and instrumentation diagrams.

Phase 2: Plant design, including the detailed mechanical design of equipment; the structural, civil, and electrical design; and the specification and design of the ancillary services. These activities will be the responsibility of specialist design groups, having expertise in the whole range of engineering disciplines.

Other specialist groups will be responsible for cost estimation and the purchase and procurement of equipment and materials.

The sequence of steps in the design, construction, and start-up of a typical chemical process plant is shown diagrammatically in Fig. 1.3, and the organization of a typical project group is shown in Fig. 1.4. Each step in the design process will not be as neatly separated from the others as is indicated in Fig. 1.3, nor will the sequence of events be as clearly defined. There will be a constant interchange of information between the various design sections as the design develops, but it is clear that some steps in a design must be largely completed before others can be started.

A project manager, often a chemical engineer by training, is usually responsible for the coordination of the project, as shown in Fig. 1.4.

As was stated in Section 1.2.1, the project design should start with a clear specification defining the product, capacity, raw materials, process, and site location. If the project is based on an established process and product, a full specification can be drawn up at the start of the project. For a new product, the specification will be developed from an economic evaluation of possible processes, based on laboratory research, pilot plant tests, and product market research. Techniques for new product design are discussed in Section 1.8.

Some of the larger chemical manufacturing companies have their own project design organizations and carry out the whole project design and engineering, and possibly construction, within their own organization. More usually, the design and construction, and possibly assistance with start-up, are subcontracted to one of the international EPC firms.

The technical "know-how" for the process could come from the operating company or could be licensed from the contractor or a technology vendor. The operating company, technology provider, and contractor will work closely together throughout all stages of the project.

On many modern projects, the operating company may well be a joint venture between several companies. The project may be carried out between companies based in different parts of the world. Good teamwork, communications, and project management are therefore critically important in ensuring that the project is executed successfully.

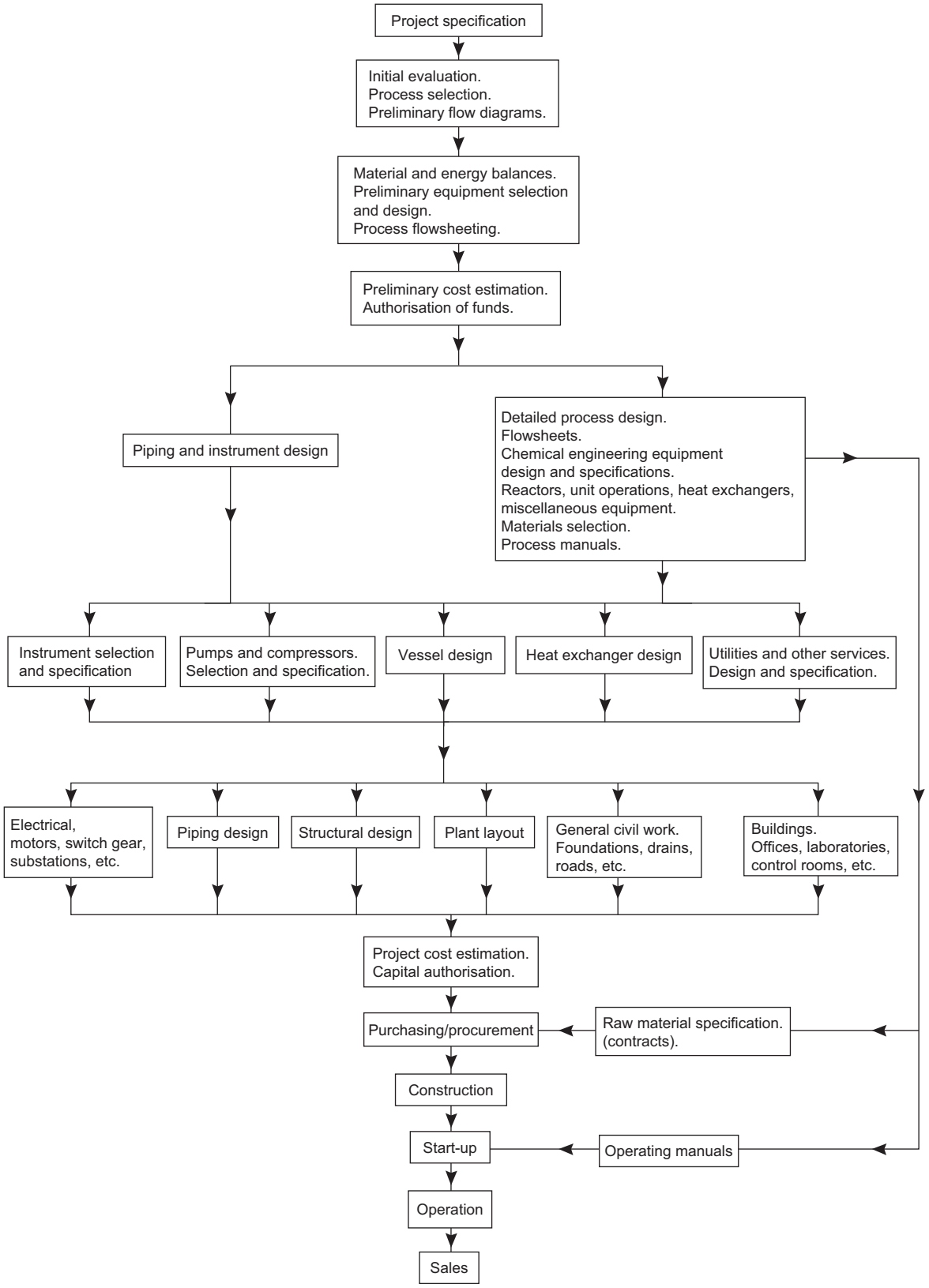


FIG. 1.3 The structure of a chemical engineering project.

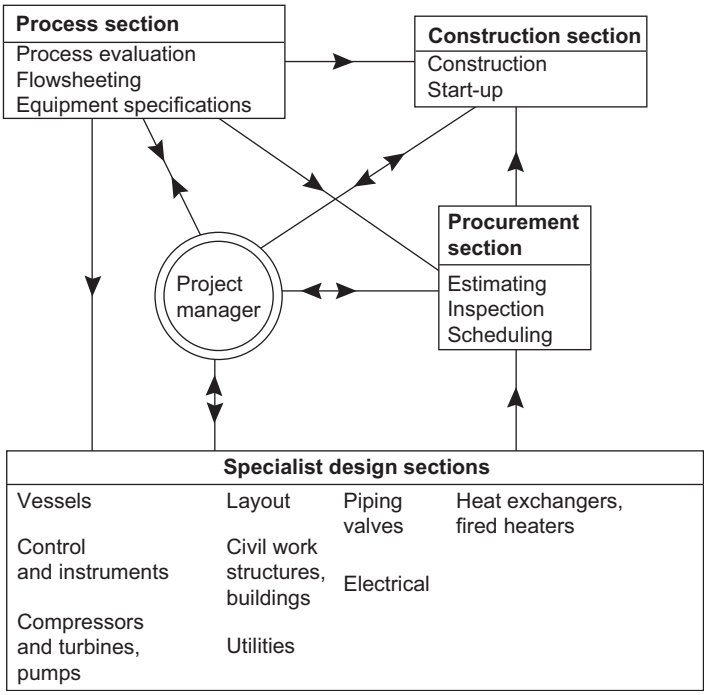


FIG. 1.4 Project organization.

1.4 Project documentation

As shown in Fig. 1.4 and described in Section 1.3, the design and engineering of a chemical process requires the cooperation of many specialist groups. Effective cooperation depends on effective communications, and all design organizations have formal procedures for handling project information and documentation. The project documentation will include:

1. General correspondence within the design group and with:
   - government departments
   - equipment vendors
   - site personnel
   - the client
2. Calculation sheets:
   - design calculations
   - cost estimates
   - material and energy balances
3. Drawings:
   - flowsheets
   - piping and instrumentation diagrams
   - layout diagrams
   - plot/site plans
   - equipment details
   - piping diagrams (isometrics)
   - architectural drawings
   - design sketches
4. Specification sheets:
   - the design basis
   - feed and product specifications
   - an equipment list
   - sheets for equipment, such as heat exchangers, pumps, heaters, etc.

5. Health, safety, and environmental information:
   - materials safety data sheets (MSDS forms)
   - HAZOP or HAZAN documentation (see Chapter 10)
   - emissions assessments and permits
6. Purchase orders:
   - quotations
   - invoices

All documents are assigned a code number for easy cross-referencing, filing, and retrieval.

1.4.1 Design documents

Calculation sheets

The design engineer should develop the habit of setting out calculations so that they can be easily understood and checked by others. It is good practice to include on calculation sheets the basis of the calculations and any assumptions and approximations made in sufficient detail for the methods, as well as the arithmetic, to be checked. Design calculations are normally set out on standard sheets. The heading at the top of each sheet should include the project title and identification number, the revision number and date, and most importantly, the signature (or initials) of the person who checked the calculation. A template calculation sheet is given in Appendix G and can be downloaded in Microsoft Excel format from the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

Drawings

All project drawings are normally drawn on specially printed sheets with the company name, project title and number, drawing title and identification number, drafter's name, and person checking the drawing clearly set out in a box in the bottom-right corner. Provision should also be made for noting on the drawing all modifications to the initial issue.

Drawings should conform to accepted drawing conventions, preferably those laid down by the national standards. The symbols used for flowsheets and piping and instrument diagrams are discussed in Chapters 2 and 5. Computer-aided design (CAD) methods are used to produce the drawings required for all aspects of a project: flowsheets, piping and instrumentation, and mechanical and civil work. Although the released versions of drawings are usually drafted by a professional, the design engineer will often need to mark up changes to drawings or make minor modifications to flowsheets, so it is useful to have some proficiency with the drafting software.

Specification sheets

Standard specification sheets are normally used to transmit the information required for the detailed design, or purchase, of equipment items, such as heat exchangers, pumps, columns, pressure vessels, etc.

As well as ensuring that the information is clearly and unambiguously presented, standard specification sheets serve as checklists to ensure that all the information required is included.

Examples of equipment specification sheets are given in Microsoft Excel format in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793. These specification sheets are referenced and used in examples throughout the book. Standard worksheets are also often used for calculations that are commonly repeated in design.

Process manuals

Process manuals are usually prepared by the process design group to describe the process and the basis of the design. Together with the flowsheets, they provide a complete technical description of the process.

Operating manuals

Operating manuals give the detailed, step-by-step instructions for operation of the process and equipment. They would normally be prepared by the operating company personnel, but may also be issued by a contractor or technology licensor as part of the technology transfer package for a less experienced client. The operating manuals are used for operator instruction and training and for the preparation of the formal plant operating instructions.

1.4.2 Design reports

Design reports are used as a means of organizing, recording, and communicating the information developed during a design project. The format of the report depends on the function of the design project. A technoeconomic analysis of a new product or process might require a strong focus on marketing and commercial aspects of the project and less technical detail, whereas a basic engineering design package that is to be used to generate a ±10% cost estimate will require substantial information on equipment designs but needs no financial analysis whatsoever.

When writing a design report, the design engineer should begin by thinking about the needs of the audience that will be using the report. Information is usually conveyed in the form of tables and charts as much as possible, with brief descriptions in the text when necessary. Most design reports are compiled from flow diagrams, specification sheets, and standard templates for economic analysis so that the technical information that users require is easily accessible. The written portion of the report is usually brief and is limited to an explanation of the key design features, assumptions, decisions, and recommendations. The following examples illustrate some of the different report formats that are commonly used in industry, and the final example discusses a suitable format for university design projects.

Example 1.1 Technoeconomic analysis

This type of report is used to summarize a preliminary technical and economic analysis of a proposed new product or process technology. Such a report might be written by an engineer working in product or process development or by a consulting company that has been asked to assess a new product or manufacturing route. This type of report is also often written as an assessment of a competitor's technology or in an effort to understand a supplier's cost structure. The purpose of the report is to provide sufficient technical and economic analysis of the process to determine whether it is economically attractive and to understand the costs of production, often in comparison with a conventional alternative. In addition to describing the technology and determining the cost of production, the report should review the attractiveness of the market and assess the risks inherent in practicing the technology. A sample contents list with guidance on each section is given in Table 1.1.

TABLE 1.1 Technoeconomic analysis

1. Executive summary (1- to 2-page summary of overall findings and recommendations, including highlights of financial analysis)
2. Technology description
   - 2.1. Process chemistry (describe the feeds, reaction mechanism, catalyst, reaction conditions, how important by-products are formed)
   - 2.2. Process specification (brief description of the process, including block flow diagram)
3. Commercial analysis
   - 3.1. Product applications (major end-use markets, competing products, legislative issues)
   - 3.2. Competitor assessment (market shares, competitor strengths, weaknesses, regional/geographic factors)
   - 3.3. Existing and planned capacity (how much and where, include plants that make feed or consume product if these have an impact on project viability—usually presented as a table)
   - 3.4. Market forecast (estimate growth rate, future price trends, regional variations in market)
   - 3.5. Project location criteria (discuss the criteria for locating a new plant, market issues, legislative factors, etc. [see Chapter 11])
4. Economic analysis
   - 4.1. Pricing basis (forecasting method, price, and/or margin assumptions)
   - 4.2. Investment analysis (explain the basis for the capital cost estimate, e.g., factorial estimate based on equipment design, curve cost estimate, etc. [see Chapter 7])
   - 4.3. Cost of production analysis (breakdown of the cost of production of product, usually presented as a table showing variable and fixed cost components [see Chapter 8])
   - 4.4. Financial analysis (evaluation of project profitability, usually presented as standard tables [see Chapter 9])
   - 4.5. Sensitivity analysis (discuss the financial impact of varying key assumptions, such as prices, plant capacity, investment cost, construction schedule [see Chapter 9])
5. Risk analysis
   - 5.1. Process hazard analysis summary (summary of critical safety issues in the design, issues raised during process hazard analysis)
   - 5.2. Environmental impact assessment summary (summary of critical environmental issues)
   - 5.3. Commercial risk assessment (discuss business risks inherent in the investment)
6. Appendices
   - 6.1. Process flow diagram
   - 6.2. Equipment list and capital cost summary

Example 1.2 Technical proposal

A technical proposal document is intended to convey the information needed to make a technology selection. When a company has decided to build a new plant, they will often invite several engineering or licensing firms to submit proposals for the plant design. Although the proposal does not contain a complete design, there must be sufficient technical information for the customer to be able to select between the proposed design and the competitor's proposals. Often, the customer will specify the contents and section headings of the proposal to ensure that all proposals follow the same format. Because the customer has already completed their own market analysis, this information is not required. Similarly, the plant capacity and location have usually already been specified. Instead, the focus of the report is on conveying the unique features of the design, the basis for selecting these features, and the proof that these features have worked in actual practice. A sample contents list is given in Table 1.2.

TABLE 1.2 Technical proposal

1. Executive summary
   - **1.1.** Proposed technology (brief description of the process, including block flow diagram)
   - **1.2.** Benefits and advantages (summarize key advantages relative to competing technologies)
2. Proposal basis
   - **2.1.** Processing objectives (restate the design problem)
   - **2.2.** Feedstocks (describe available feedstocks, grades, quality issues)
   - **2.3.** Product grades (give product specifications, usually as tables or reference to ASTM specifications)
   - **2.4.** Processing options (describe technical alternatives evaluated)
3. Proposed technology
   - **3.1.** Process description (more detailed process description)
   - **3.2.** Reactor selection (what reactor type is recommended, why it was selected, and how it was designed)
   - **3.3.** Catalyst selection recommendations (what catalysts are recommended and why)
   - **3.4.** Key equipment recommendations (describe any critical unit operations and explain what was selected and how it was designed, key specifications, etc.)
   - **3.5.** Pilot plant and commercial experience (describe any work that proves that the proposed design will operate as described)
4. Technical and economic assessment
   - **4.1.** Estimated raw materials consumption (usually a table)
   - **4.2.** Estimated utility consumption (usually a table giving breakdowns for each utility [see Chapter 3])
   - **4.3.** Estimated manpower requirements (how many operators are needed per shift)
   - **4.4.** Estimated cost of production (breakdown of the cost of production of product, usually presented as a table showing variable and fixed cost components [see Chapter 8])
   - **4.5.** Estimated installed capital cost (breakdown by plant section of the plant capital cost estimate)
5. Process flow diagrams
6. Preliminary equipment specification sheets
7. Typical plot plan

Example 1.3 Basic engineering design

A basic engineering design report (BEDR) is often used at the end of the process design phase to collect and review information before beginning the plant design phase and detailed design of equipment, piping, plot layout, etc. The purpose of the BEDR is to ensure that all the information necessary for detailed design has been assembled, reviewed, and approved so as to minimize errors and rework during detailed design. The BEDR also serves as a reference document for the detailed design groups and provides them with stream flows, temperatures, pressures, and physical property information. One of the most important functions of a basic engineering design report is to document the decisions and assumptions made during the design and the comments and suggestions made during design review meetings. These are often documented as separate sections of the report so that other engineers who later join the project can understand the reasons why the design evolved to its current form. A sample contents list for a basic engineering design report is given in Table 1.3.

TABLE 1.3 Basic engineering design

1. Process description and basis
   - 1.1. Project definition (customer, location, key feeds, and products)
   - 1.2. Process description (brief description of process flowsheet and chemistry, including block flow diagrams)
   - 1.3. Basis and scope of design (plant capacity, project scope, design basis table)
2. Process flow diagrams
3. Mass and energy balances
   - 3.1. Base case stream data (stream temperature and pressure, mass flow and molar flow of each component in all streams, stream mass and molar composition, and total stream mass and molar flow, usually given as tables)
   - 3.2. Modified cases stream data (same data for each variant design case, for example, winter/summer cases, start of run/end of run, different product grades, etc.)
   - 3.3. Base case physical property data (physical properties required by detailed design groups, such as stream density, viscosity, thermal conductivity, etc.)
4. Process simulation (description of how the process was simulated and any differences between the simulation model and process flow diagram that detailed design groups need to understand)
5. Equipment list
6. Equipment specifications
   - 6.1. Pressure vessels
   - 6.2. Heaters
   - 6.3. Heat exchangers
     - 6.3.1. Tubular
     - 6.3.2. Air cooled
   - 6.4. Fluid handling equipment
     - 6.4.1. Pumps
     - 6.4.2. Compressors
   - 6.5. Solid handling equipment
   - 6.6. Drivers
     - 6.6.1. Motors
     - 6.6.2. Turbines
   - 6.7. Unconventional or proprietary equipment
   - 6.8. Instrumentation
   - 6.9. Electrical specifications
   - 6.10. Piping
   - 6.11. Miscellaneous
7. Materials of construction (what materials are to be used in each section of the plant and why they were selected, often presented as a table or as a marked-up version of the process flow diagram)
8. Preliminary hydraulics (pump-and-line calculations of pressure drop used as a basis for sizing pumps and compressors [see Chapter 20])
9. Preliminary operating procedures (describe the procedures for plant start-up, shut-down, and emergency shut-down)
10. Preliminary hazard analysis (description of major materials and process hazards of the design [see Chapter 10])
11. Capital cost estimate (breakdown of capital cost, usually for each piece of equipment plus bulks and installation, usually given as a table or list)
12. Heat integration and utilities estimate (overview of any pinch analysis or other energy optimization analysis, composite curves, table giving breakdown of utility consumption and costs [see Chapter 3])
13. Design decisions and assumptions (description of the most significant assumptions and selection decisions made by the designers, including references to calculation sheets for alternatives that were evaluated and rejected)
14. Design review documentation
    - 14.1. Meeting notes (notes taken during the design review meeting)
    - 14.2. Actions taken to resolve design review issues (description of what was done to follow up on issues raised during the design review)
15. Appendices
    - 15.1. Calculation sheets (calculations to support equipment selection and sizing, numbered and referenced elsewhere in the report)
    - 15.2. Project correspondence (communications between the design team, marketing, vendors, external customers, regulatory agencies, and any other parties whose input influenced the design)

Example 1.4 Undergraduate design project

Senior-year design projects have a range of objectives, but these always include demonstrating proficiency in engineering design and economic evaluation. More technical information is needed than in Example 1.1, whereas more commercial and marketing analysis is needed than in Examples 1.2 and 1.3, so none of the report formats used in industry is ideal. A reasonable approach is to use the format of Example 1.1 and include the material listed in Example 1.3 as appendices. For shorter classes, or when there is insufficient time to develop all the information listed in Example 1.3, some of the sections of Table 1.3 can be omitted.

1.5 Codes and standards

The need for standardization arose early in the evolution of the modern engineering industry; Whitworth introduced the first standard screw thread to give a measure of interchangeability between different manufacturers in 1841. Modern engineering standards cover a much wider function than the interchange of parts. In engineering practice, they cover:

1. Materials, properties, and compositions
2. Testing procedures for performance, compositions, and quality
3. Preferred sizes; for example, tubes, plates, sections, etc.
4. Methods for design, inspection, and fabrication
5. Codes of practice for plant operation and safety

The terms *standard* and *code* are used interchangeably, though *code* should really be reserved for a code of practice covering, say, a recommended design or operating procedure, and *standard* for preferred sizes, compositions, etc.

All of the developed countries, and many of the developing countries, have national standards organizations responsible for the issue and maintenance of standards for the manufacturing industries and for the protection of consumers. In the United States, the government organization responsible for coordinating information on standards is the National Institute of Standards and Technology (NIST); standards are issued by federal, state, and various commercial organizations. The principal ones of interest to chemical engineers are those issued by the American National Standards Institute (ANSI), the American Petroleum Institute (API), the American Society for Testing Materials (ASTM), the American Society of Mechanical Engineers (ASME) (pressure vessels and pipes), the National Fire Protection Association (NFPA) (safety), the Tubular Exchanger Manufacturers Association (TEMA) (heat exchangers), and the Instrumentation, Systems and Automation Society (ISA) (process control). Most Canadian provinces apply the same standards used in the United States. The preparation of the standards is largely the responsibility of committees of persons from the appropriate industry, the professional engineering institutions, and other interested organizations.

The International Organization for Standardization (ISO) coordinates the publication of international standards. The European countries used to each maintain their own national standards, but these are now being superseded by common European standards.

Lists of codes and standards and copies of the most current versions can be obtained from the national standards agencies or by subscription from commercial websites such as IHS (www.ihs.com).

As well as the various national standards and codes, the larger design organizations will have their own (in-house) standards. Much of the detail in engineering design work is routine and repetitious, and it saves time and money, and ensures conformity between projects, if standard designs are used whenever practicable.

Equipment manufacturers also work to standards to produce standardized designs and size ranges for commonly used items, such as electric motors, pumps, heat exchangers, pipes, and pipe fittings. They will conform to national standards, where they exist, or to those issued by trade associations. It is clearly more economic to produce a limited range of standard sizes than to have to treat each order as a special job.

For the designer, the use of a standardized component size allows for the easy integration of a piece of equipment into the rest of the plant. For example, if a standard range of centrifugal pumps is specified, the pump dimensions will be known, and this facilitates the design of the foundation plates, pipe connections, and selection of the drive motors: standard electric motors would be used.

For an operating company, the standardization of equipment designs and sizes increases interchangeability and reduces the stock of spares that must be held in maintenance stores.

Though there are clearly considerable advantages to be gained from the use of standards in design, there are also some disadvantages. Standards impose constraints on the designer. The nearest standard size will normally be selected on completing a design calculation (rounding up), but this will not necessarily be the optimum size, though; as the standard size will be cheaper than a special size, it will usually be the best choice from the point of view of initial capital cost. The design methods given in the codes and standards are, by their nature, historical and do not necessarily incorporate the latest techniques.

The use of standards in design is illustrated in the discussion of pressure vessel design in Chapter 14 and the description of heat exchanger design in Chapter 19. Relevant design codes and standards are cited throughout the book.

1.6 Design factors (design margins)

Design is an inexact art; errors and uncertainties arise from uncertainties in the design data available and in the approximations necessary in design calculations. Experienced designers include a degree of overdesign known as a *design factor, design margin,* or *safety factor* to ensure that the design that is built meets product specifications and operates safely.

In mechanical and structural design, the design factors that are used to allow for uncertainties in material properties, design methods, fabrication, and operating loads are well established. For example, a factor of around 4 on the tensile strength, or about 2.5 on the 0.1% proof stress, is normally used in general structural design. The recommended design factors are set out in the codes and standards. The selection of design factors in mechanical engineering design is illustrated in the discussion of pressure vessel design in Chapter 14.

Design factors are also applied in process design to give some tolerance in the design. For example, the process stream average flows calculated from material balances are usually increased by a factor, typically 10%, to give some flexibility in process operation. This factor will set the maximum flows for equipment, instrumentation, and piping design. Where design factors are introduced to give some contingency in a process design, they should be agreed within the project organization and clearly stated in the project documents (drawings, calculation sheets, and manuals). If this is not done, there is a danger that each of the specialist design groups will add its own "factor of safety," resulting in gross and unnecessary overdesign. Companies often specify design factors in their design manuals.

When selecting the design factor, a balance has to be made between the desire to make sure the design is adequate and the need to design to tight margins to remain competitive. Greater uncertainty in the design methods and data requires the use of bigger design factors.

1.7 Systems of units

Most of the examples and equations in this book use SI units; however, in practice the design methods, data, and standards that the designer will use are often only available in the traditional scientific and engineering units. Chemical engineering has always used a diversity of units, embracing the scientific CGS and MKS systems and both the American and British engineering systems. Those engineers in the older industries will also have had to deal with some bizarre traditional units, such as degrees Twaddle or degrees API for density and barrels for quantity. Although almost all of the engineering societies have stated support for the adoption of SI units, this is unlikely to happen worldwide for many years. Furthermore, much useful historic data will always be in the traditional units, and the design engineer must know how to understand and convert this information. In a globalized economy, engineers are expected to use different systems of units even within the same company, particularly in the contracting sector, where the choice of units is at the client's discretion. Design engineers must therefore have a familiarity with SI, metric, and customary units, and a few of the examples and many of the exercises are presented in customary units.

It is usually best practice to work through design calculations in the units in which the result is to be presented, but if working in SI units is preferred, data can be converted to SI units, the calculation made, and the result converted to whatever units are required. Conversion factors to the SI system from most of the scientific and engineering units used in chemical engineering design are given in Appendix D, which is at the end of this book as well as in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

Some license has been taken in the use of the SI system in this volume. Temperatures are given in degrees Celsius (°C); degrees Kelvin are only used when absolute temperature is required in the calculation. Pressures are often given in bar (or atmospheres) rather than in Pascals (N/m^2), as this gives a better feel for the magnitude of the pressures. In design calculations the bar can usually be taken as equivalent to an atmosphere, whatever definition is used for atmosphere. The abbreviations bara and barg are often used to denote bar absolute and bar gauge, analogous to psia and psig when the pressure is expressed in pound force per square inch. When bar is used on its own, without qualification, it is normally taken as absolute.

For stress, N/mm^2 have been used, as these units are now generally accepted by engineers, and the use of a small unit of area helps indicate that stress is the intensity of force at a point (as is pressure). The corresponding traditional unit for stress is the ksi, or thousand pounds force per square inch. For quantity, kmol are generally used in preference to mol, and for flow, kmol/h instead of mol/s, as this gives more sensibly sized figures, which are also closer to the more familiar lb/h.

For volume and volumetric flow, m^3 and m^3/h are used in preference to m^3/s, which gives ridiculously small values in engineering calculations. Liters per second are used for small flow rates, as this is the preferred unit for pump specifications.

Plant capacities are usually stated on an annual mass flow basis in metric tons per year. Unfortunately, the literature contains a variety of abbreviations for metric tons per year, including tonnes/y, metric tons/y, MT/y (also kMTA = thousand metric tons per year), mtpy, and the correct term, t/y. The nonstandard abbreviations have occasionally been used, as it is important for design engineers to be familiar with all of these terms. The unit t denotes a metric ton of 1000 kg. In this book the unit ton is generally used to describe a short ton or U.S. ton of 2000 lb (907 kg) rather than a long ton or UK ton of 2240 lb (1016 kg), although some examples use long tons. The long ton is closer to the metric ton. A thousand metric tons is usually denoted as a kiloton (kt); the correct SI unit gigagram (Gg) is rarely used.

In the United States, the prefixes M and MM are often used to denote thousand and million, which can be confusing to anyone familiar with the SI use of M as an abbreviation for *mega* ($\times 10^6$). This practice has generally been avoided, except in the widely used units MMBtu (million British thermal units) and the common way of abbreviating $1 million as $1 MM.

Most prices have been given in U.S. dollars, denoted US$ or $, reflecting the fact that the data originated in the United States.

Where, for convenience, other than SI units have been used on figures or diagrams, the scales are also given in SI units, or the appropriate conversion factors are given in the text. Where equations are presented in customary units, a metric equivalent is generally given.

Some approximate conversion factors to SI units are given in Table 1.4. These are worth committing to memory to give some feel for the units for those more familiar with the traditional engineering units. The exact conversion factors are also shown in the table. A more comprehensive table of conversion factors is given in Appendix D.

TABLE 1.4 Approximate conversions between customary units and SI units

		SI Unit	
Quantity	**Customary Unit**	**Approx.**	**Exact**
Energy	1 Btu	1 kJ	1.05506
Specific enthalpy	1 Btu/lb	2 kJ/kg	2.326
Specific heat capacity	1 Btu/lb°F	4 kJ/kg°C	4.1868
Heat transfer coeff.	1 Btu/ft^{2}h°F	6 W/m^2°C	5.678
Viscosity	1 centipoise	1 mNs/m^2	1.000
	1 lb$_f$/ft h	0.4 mNs/m^2	0.4134
Surface tension	1 dyne/cm	1 mN/m	1.000
Pressure	1 lbf/in^2 (psi)	7 kN/m^2	6.894
	1 atm	1 bar	1.01325
		10^5 N/m^2	
Density	1 lb/ft^3	16 kg/m^3	16.0185
	1 g/cm^3	1 kg/m^3	
Volume	1 US gal	3.8×10^{-3} m^3	3.7854×10^{-3}
Flow-rate	1 US gal/min	0.23 m^3/h	0.227

Note:
1US gallon = 0.84 imperial gallons (UK)
1barrel (oil) = 42 US gallons ≈ 0.16 m^3 (exact 0.1590)
1kWh = 3.6 MJ

1.8 Product design

The design of new chemical products goes through the same stages described in Section 1.2 and illustrated in Fig. 1.2. The successful introduction of a new product usually requires not only the design of the product itself but also the design of the plant that will make the product. In the process industries the conception and development of new chemical products are often led by chemists, biologists, pharmacists, food scientists, or electrical or biomedical engineers; however, chemical engineers can be involved from the earliest stages and will certainly be engaged in designing the manufacturing process and developing the first estimates of the cost of production and capital investment required.

The launch of a new product always has high commercial risk. The new product must meet a customer need and outperform the existing alternatives. Customers may have multiple requirements of the product, and these requirements may not be stated in a way that is easy to relate to technical specifications. The company that introduces the product needs to build market share and command a high enough price to ensure that the investment in research, development, and a new plant can be justified.

Most of the engineering work that is done in launching a new product goes into the design of the manufacturing process, but considerable care must be taken to ensure that the commercial risks have also been properly addressed. Consequently, in new product design much more attention is paid to the steps of understanding customer preferences, translating these needs into product specifications, and market testing to ensure fitness for service.

This section introduces some of the methods that are used for product development in the process industries and that may be useful to chemical engineers engaged in new product design. Vast quantities of books on innovation and new product design have been published in the general engineering and business literature. Among the best are those by Cooper (2017), Ulrich et al. (2020), and Cooper and Edgett (2009). Product design books aimed specifically at chemical engineers have been written by Cussler and Moggridge (2011) and Seider et al. (2016).

1.8.1 New Chemical Products

Chemical engineers work in many industries and may be engaged in designing all kinds of products, but for the purposes of this chapter the discussion will be limited to new products that are based on the application of novel chemistry, biology, or materials science. These can be broadly categorized as new molecules, new formulations, new materials, and new equipment and devices.

New molecules

The process industries produce and consume a surprisingly large number of distinct chemical species. Under the Toxic Substances Control Act of 1976 (TSCA) (15 U.S.C. 2601 *et seq*.), the U.S. Environmental Protection Agency (EPA) regulates the manufacture, import, and export of 83,000 chemicals. The European Chemicals Agency (ECHA) was established in 2006 under the European Regulation, Evaluation, Authorization and Restriction of Chemicals (REACH) regulation, with the goal of registering all chemicals in use in Europe. At the time of writing, 143,000 chemicals have been submitted to ECHA for pre-registration. The infinite possibilities of organic chemistry ensure that we will never run out of new molecular species to test for any given application.

New molecules are often commercialized in high-value applications such as specialty chemicals, additives, and active pharmaceutical ingredients (APIs). New molecules may also be needed when use of an existing chemical is restricted for safety or environmental reasons. For example, chlorinated hydrocarbons were phased out as refrigerants and propellants under the Montreal Protocol after concern that they caused ozone depletion. The fluorocarbon compounds that replaced them are in turn likely to be replaced due to concerns about their high global-warming potential as greenhouse gases.

Various methods are used to identify new molecules for an application. Optimization of computer models based on molecular simulation or group contribution methods may provide insights into molecular structures that give desired properties. More often, chemists will look at variants on known molecules, for example, by addition, removal, or substitution of methyl-, ethyl-, phenyl- or other substituent groups. The chemists will also use their knowledge of synthesis routes to propose compounds that are easier to prepare in high yield using known chemical pathways and starting from available feeds. The same is true for biologically derived compounds, where the biochemist or genetic engineer will attempt to isolate enzymes or strains that maximize the yield of the target molecule.

New formulations

Almost all process industry products sold to the general public are formulations made from multiple chemicals. Examples range from pharmaceuticals, cosmetics, healthcare products, fragrances, foods, and beverages to paints, adhesives, fuels, and cleaning products. Every household contains a multitude of mixtures of products.

The prevalence of formulated products arises directly from the need to meet multiple customer requirements. You can wash your hands quite effectively using linear alkylbenzene sulfonate (a surfactant), but you probably prefer it to be blended into a gel that smells nice, has an attractive color, and provides some antibacterial action. The same surfactant would also be quite suitable for washing your car, clothes, dishes, carpets, hair, and toilet, but in each case specific user requirements lead to a different formulated product.

Formulated products are usually produced in blending plants. In some simple cases the feed compounds are just mixed together and sent to a packaging line. More commonly, the mixing and blending operations must be carefully designed to ensure (or prevent) emulsification and guarantee uniform product properties. Formulation plants are also often designed to produce a range of different products tailored to different market segments, in which case the plant must be designed to switch between products with minimal downtime and product wastage.

The blend composition of a formulated product is designed to meet the customer needs in a cost-effective manner that provides an adequate profit margin for the manufacturer. Where possible, manufacturers seek to substitute expensive components with cheaper materials that have the same effect; however, marketing and brand management can sometimes be used to justify using more expensive materials. For example, "natural" compounds derived from agricultural products can often be effectively marketed to replace cheaper synthetic alternatives.

Consumer products are highly regulated and carry high potential liability risks because of the large number of end users. These factors place additional constraints on the product designers. Extensive product safety testing must be carried out when new chemicals are introduced into consumer product formulations.

New materials

Chemical engineers play a leading role in the manufacture of polymers, synthetic fibers, composite materials, papers, films, electronic materials, catalysts, and ceramics. The properties of these materials are often determined as much by the manufacturing process as by the chemical composition. For example, multiple grades of polyethylene can be produced, with very different properties, depending on the production route and distribution of molecular weight in the polymer.

New product development in the manufacturing industries is often based on materials substitution. Injection-molded or film-blown polymers are usually a cheaper substitute for metal, wood, or glass components that require more labor-intensive casting or machining. Many chemical engineers work on tailoring the properties of engineering materials such as polymers, resins, and composites to optimize the material to particular end applications.

The development of new materials applications requires close collaboration with the end user of the material. Most of the product specifications will be based on physical properties such as strength, elasticity, hardness, etc., and flow properties that affect ease of manufacture, but resistance to chemicals, solvents, oxidation, and corrosion can also be important factors.

New equipment and devices

Many sensors, medical devices, and power systems are based on chemical or biological processes. If a device requires sound understanding of kinetics and transport processes, chemical engineers will probably be involved in its design. Chemical engineers also play an important role in the design of new proprietary equipment for the processing industries and are frequently involved in the design and customization of equipment such as dryers, crystallizers, membrane units, and other proprietary separation devices.

Device manufacture usually involves the assembly of multiple subcomponents, and the production line methods that are used are very different from the methods used in the process industries. Evaluating the production costs of manufactured devices requires familiarity with industrial engineering methods and is beyond the scope of this book.

1.8.2 Understanding customer needs

The first step in new product development is to find out what customers want and are prepared to pay for. If the new product is not better than existing alternatives in some way, then it will be difficult to build market share and generate a return on the investment. If new features are added, they must be of value to the customer; otherwise, the new product will not be differentiated from the existing alternatives. One of the roles of the marketing group in a company is to develop an understanding of customer requirements and willingness to spend and use this understanding to guide new product development teams.

The level of market research that is needed depends on the nature of the product and the homogeneity of the customer base. In some cases, the customers may all have very similar needs. For example, when UOP developed a renewable jet fuel based on hydrotreated vegetable oils, it was clear that the product must meet all the standard ASTM specifications for jet fuels. More often, however, the customers fall into different groups, known as *market segments*, each with different requirements. The product development team must consider the needs of each segment and determine whether a product can be designed to meet the needs of several segments or whether it is necessary to develop customized products for each segment.

It is important to distinguish between proximate and ultimate customers when carrying out market research. Many chemical products are sold to other manufacturers (proximate customers) who then incorporate the chemical product into their own products to sell to end users (ultimate customers). Some product features may be very valuable to the proximate customer while having little value to the ultimate customer. Improving the processability, handling, storage, or safety properties of a product will make it easier and potentially cheaper to use, but may have little effect on its end-use application. For example, a paint composition with a faster drying time may be attractive to an automobile manufacturer, but will not be noticed by the customer who buys the car.

Many methods have been developed for market research. Interviews and customer conferences can be used when the number of customers is small or when a representative sample group can be assembled. When the customer base is large and diverse, manufacturers use surveys and focus groups. The questions that are posed in market research studies must be carefully formulated so as to not only discover customer preferences but also identify latent needs that are not met by the existing products. Ulrich et al. (2020) suggest the following generic questions that can be used in interviews or focus groups:

- When and why do you use this product?
- What do you like about the existing products?
- What do you dislike about the existing products?
- What issues do you consider when purchasing the product?
- What improvements would you make to the product?

In addition to finding customer needs, good market research studies determine the relative importance of different needs and the willingness of the customer to pay for certain features. As the new product undergoes development, it may be necessary to repeat the market research to validate the product concept and test how well it meets customer expectations.

1.8.3 Developing product specifications

The needs stated by customers in the marketing study are usually not expressed in terms of technical product specifications. The design team must translate these needs into measurable properties of the product and then set a target value or range for each property. Product specifications must reflect all of the following factors:

- Product safety and regulatory requirements
- Potential liability concerns
- Fitness for purpose
- Customer needs and preferences
- Marketing advantages
- Maximization of profit margin

When setting specifications, it is important to remember that a specification should tell you *what* the product does, but not *how* it does it. For example, a customer need for a beverage such as a milk shake is to have the right "mouth feel." One way to accomplish this might be by setting a specification on viscosity. The design team could then modify the recipe to meet the viscosity specification in many different ways. It would not be as effective to set a specification on xanthan gum concentration, as this presupposes the use of a particular thickener and overconstrains the design of the product.

Regulations and standards can be important sources of specifications. If a product is subject to regulation, then all the regulated specifications must be met, and new features can only be introduced if they do not require regulation or have obtained the necessary approval. Product safety, disposal, and environmental impact considerations can also lead to specifications that may not have been articulated by the customers. It is also important for the design team to consider potential product liability. The fact that a product is not currently regulated does not mean that it is safe,

and if there are concerns about public health or safety, then these should be raised and properly evaluated so that the company can assess the potential for future litigation.

Quality function deployment

A method that is widely used in translating customer needs into specifications is *Quality Function Deployment* (QFD) (Hauser and Clausing, 1988). Several variations of the QFD method have been developed, but all are based on the concept of relating customer needs to product specifications and comparing the proposed product to the existing competitors.

A QFD analysis is set out as a table or matrix and is usually carried out using a spreadsheet. Examples of simple QFD tables are given in Figs. 1.5 and 1.6. The first column lists the customer needs identified by the market research study. Each customer need is assigned a priority or importance, P, which is usually an integer on a 1 to 10 scale, based on the customer feedback. In some versions of the method a measure or metric is assigned to each customer need; however, this is not always necessary. The design team then lists all the product specifications that they envision and enters each specification as a column in the table. The team assigns a score, s, to how strongly each specification affects each customer need. A typical scoring scale might be 3 = critical, 2 = strong, 1 = weak, and 0 = no impact. The scores are multiplied by the corresponding customer priority and summed to give an overall relative importance of each specification, which is entered at the bottom of each column:

$$\text{Relative importance of specification } i = \sum_j P_j\, s_{ij} \tag{1.1}$$

Where: P_j = customer priority assigned to need j
s_{ij} = score for how well specification i meets need j

In some cases, additional columns are added to the right of the table for the existing competing products, as shown in Fig. 1.5. Each existing product can be assigned a score, c, for how well it meets each customer need, using the same scoring scale used for the specifications. These scores can also be multiplied by the corresponding customer priority and summed to give an indication of the relative strength of the existing products.

The QFD exercise has several uses. It helps the design team identify which specifications correlate most strongly with each customer need, and hence focuses effort on the aspects of the product that customers value most. If none of the specifications has a high score against a particular need, then it can highlight the need for new features or specifications. It can help identify strengths and weaknesses in competitors' products and identify which specifications must be adjusted to give superior performance to the competition. Lastly, it can help identify specifications that have an impact on multiple customer needs and potentially lead to trade-offs between different customer desires.

Customer needs	Priority	Specification 1	Specification 2	Specification 3	Specification 4	Specification 5	Specification 6	Competing product 1	Competing product 2	Competing product 3	Competing product 4	Competing product 5
Need 1	P_1	s_{11}	s_{21}	s_{31}	s_{41}	s_{51}	s_{61}	c_{11}	c_{21}	etc.		
Need 2	P_2	s_{12}	s_{22}	s_{32}	s_{42}	s_{52}	s_{62}	c_{12}	c_{22}			
Need 3	P_3	s_{13}	s_{23}	s_{33}	s_{43}	s_{53}	s_{63}	c_{13}	c_{23}			
etc.												
Relative importance		$\Sigma P_j S_{ij}$	etc.									

P_j = priority assigned to need j by customer
s_{ij} = score for how well specification i meets need j
c_{ij} = score for how well competing product i meets need j

FIG. 1.5 QFD table.

Customer needs	Priority	Abrasive content	Fluoride content	Non-sugar sweetener	Flavor content	Viscosity modifier	Solid thickener	Antiseptic content	Bleach content
Cleans teeth	8	3	0	0	0	0	0	1	0
Removes plaque	9	3	0	0	0	0	0	0	0
Whitens teeth	5	0	0	0	0	0	0	0	3
Tastes fresh	6	0	0	3	3	1	1	2	1
Freshens breath	7	0	0	0	3	0	0	2	1
Squeezes out right	5	2	0	0	0	3	3	0	0
Not gritty	6	3	0	0	0	0	2	0	0
Strengthens teeth	8	0	3	0	0	0	0	0	0
Prevents gingivitis	9	0	0	0	0	0	0	3	0
Relative Importance		79	24	18	39	21	33	61	28

FIG. 1.6 Completed QFD for toothpaste.

A simplified example of a QFD analysis is given in Example 1.5. More information on details of the method is given in the book by Ulrich et al. (2020) and the article by Hauser and Clausing (1988). The QFD method has become very widely used as part of the Six Sigma methodology; see Pyzdek and Keller (2018) for more on Six Sigma.

Example 1.5. QFD analysis

Complete a QFD analysis to determine the important specifications for a toothpaste product.

Solution

One possible solution is shown in Fig. 1.6. A market survey (with a very limited set of customers) identified the following customer needs for toothpaste: cleans teeth, removes plaque, whitens teeth, tastes fresh, freshens breath, squeezes out right, not gritty, strengthens teeth, and prevents gingivitis. These are entered in the first column, with the relative priorities listed in the second column.

Some possible product specifications are then listed as additional columns. These include abrasive content, fluoride content, non-sugar sweetener, flavor content, viscosity modifier, solid thickener, antiseptic content, and bleach content. Note that these specifications do not specify the use of a particular bleach, sweetener, flavor, etc., so the designers might be able to meet several specifications using the same compound.

The scores are then entered for each specification. For example, the abrasive content is critical for "cleans teeth" and "removes plaque" (score 3 in both cases) but has no effect on "whitens teeth," "tastes fresh," or "freshens breath" (score 0). The abrasive content can have a strong effect on how the paste squeezes (score 2) and can have a critical impact on "not gritty" (score 3). Note that in this last case, the impact is negative and the customer desire for a particular mouth feel in the product is somewhat at odds with improving product performance.

The relative importance of the specification is then calculated as the priority-weighted sum of the scores, using Equation 1.1.

$$\begin{aligned}\text{Relative importance for abrasive content} &= 8(3) + 9(3) + 5(2) + 6(3) \\ &= 24 + 27 + 10 + 18 = 79\end{aligned}$$

Scores are then assigned to how well every other specification meets each need until the table is completed.

Reviewing the completed table, we can see that all of the specifications have a critical impact on at least one of the customer needs and some have an impact on several needs. The abrasive content clearly has a strong impact on product performance and also on "not gritty," so one conclusion of the QFD study might be to focus on examining different abrasive materials or different particle size distributions of abrasive so as to attempt to strike a better balance between these conflicting needs.

1.8.4 Fitness testing

As the design team develops potential product concepts, they will need to test each concept to determine how well it meets the desired specifications. In the cases of new molecules and new materials, testing will usually consist of synthesizing the material and carrying out experiments to determine its properties. For new equipment and formulations, more extensive prototyping and customer validation of the benefits of the design may be needed.

Prototype testing

Engineers build prototypes to address several different aspects of new product development:

- If new features are introduced in the design, it may be necessary to build a prototype to test these features and make sure that they work properly and safely.
- When a product is assembled from many components, it may be necessary to build a prototype to ensure that all the components work together properly when integrated as a system.
- The assembly of a prototype helps the designers understand the manufacturing process for the final product and can highlight features of the design that will make manufacturing easy or difficult. Prototyping is thus an important step in *design for manufacture.*
- In the design of formulated products, the manufacturer will often want to evaluate whether a component can be substituted with a cheaper material that has similar properties. It may be necessary to prepare alternative versions of the formulation with each component so that they can be tested side by side for properties and customer acceptance.
- A prototype can be used as a communication device to demonstrate features of a design. It can therefore be used to validate design features with potential customers or with management and hence confirm the marketing advantages of the new design.

Prototypes can take many forms, depending on the product type and stage of development. In the early stages of product development, conceptual or computer models are widely used. Working models of subcomponents are usually easier to test than full products; however, a full physical working model or exact recipe must usually be created for final product testing. Note that the activity of prototyping is not restricted to equipment and devices: testing different formulations of shampoo or cookie dough accomplishes the same goals.

Before a prototype is built, the design team should have a clear idea of the purpose of the prototype and the testing or experiments for which it will be used. Engineers from the manufacturing plant should be engaged as part of the development team to ensure that manufacturability concerns are flushed out and addressed. Several iterations of prototyping may need to be planned before a final product design can be selected.

Safety and efficacy testing

One of the most rigorous new product testing processes is the procedure used for obtaining approval from the U.S. Food and Drug Administration (FDA) for new medicines. The evaluation process is designed to ensure both the safety and efficacy of new drugs. If a company believes it has developed a new molecule with a therapeutic application, then it must go through the following steps:

- *Preclinical trials*: Initial testing on enzymes or cells in a laboratory, followed by animal tests usually on at least two species.
- *Phase I studies*: Testing on a small number of healthy volunteers (often medical students!) to ensure the treatment is safe.
- *Phase II studies*: Testing on patients who have the same disease or condition that is to be treated to evaluate efficacy at different dose levels.
- *Phase III studies*: Testing on a large number (hundreds or thousands) of patients who have randomly been assigned either the drug or a placebo to validate the efficacy of the treatment and assess possible side effects and interactions with other medications.

The results of the clinical trials are reviewed by an independent FDA panel to determine if the benefits of treatment outweigh the risks posed by any observed side effects. The entire process typically takes over 8 years and can cost more than $800 million (DiMasi et al., 2003; FDA, 2006). Even when the product is approved, the manufacturer must still submit to FDA inspections to ensure that quality control procedures are adequate and the production facility complies with FDA current good manufacturing practices (cGMP). Additional information on GMP requirements is given in the discussion of bioreactor quality control in Section 15.9.8.

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1.10 Nomenclature

		Dimensions in $MLT\theta$
c_{ij}	Score for how well competing product i meets customer need j	—
P_j	Priority assigned by customer to need j	—
s_{ij}	Score for how well specification i meets customer need j	—

1.11 Problems

1.1 Develop project plans for the design and construction of the following processes. Use Fig. 1.2 as a guide to the activities that must occur. Estimate the overall time required from launching the project to the start of operation.
a. A petrochemical process using established technology to be built on an existing site.
b. A process for full-scale manufacture of a new drug, based on a process currently undergoing pilot plant trials.
c. A novel process for converting cellulose waste to fuel products.
d. A spent nuclear fuel reprocessing facility.
e. A solvent recovery system for an electronics production facility.

1.2 You are the project manager of a team that has been asked to complete the design of a chemical plant up to the stage of design selection. You have three engineers available (plus yourself), and the work must be completed in 10 weeks. Develop a project plan and schedule of tasks for each engineer. Be sure to allow sufficient time for equipment sizing, costing, and optimization. What intermediate deliverables would you specify to ensure that the project stays on track?

1.3 You are part of a product design team that has been asked to develop a low-calorie chocolate chip cookie dough.
a. Poll your classmates to determine customer requirements.
b. Carry out a QFD analysis to map the customer requirements into product specifications

CHAPTER

2

Process flowsheet development

KEY LEARNING OBJECTIVES

- How to read and draw a process flow diagram (PFD)
- When to design a batch process or a continuous process
- Factors to consider when adopting or improving commercially proven technology
- How to develop a flowsheet for a revamp design
- How to synthesize a flowsheet for an entirely new process
- How to review a flowsheet and check for completeness and errors

2.1 Introduction

This chapter covers the preparation and presentation of the process flowsheet, also known as the *process flow diagram (PFD)*. The flowsheet is the key document in process design. It shows the arrangement of the equipment selected to carry out the process, the stream connections, the stream flow rates and compositions, and the operating conditions. It is a diagrammatic model of the process. Chemical engineers in industry are usually very proficient at reading PFDs and use it as the primary means of transmitting and recording process information.

The flowsheet is used by specialist design groups as the basis for their designs. These include piping, instrumentation, and equipment design and plant layout. It is also used by operating personnel for the preparation of operating manuals and operator training. During plant start-up and subsequent operation, the flowsheet forms a basis for the comparison of operating performance with design. If the plant is later revamped to new specifications, the PFD of the original plant is the starting point for the revamp design.

Several types of PFDs are used by chemical engineers, depending on the level of detail required. A simple block flow diagram can be used to give a rough idea of the overall process flow structure and may be useful when giving a presentation. A full PFD should include all of the process vessels and equipment and show all the process and utility flow lines. A full heat and material balance of the process showing the composition, flow rate, and temperature of every stream is usually included in or with a PFD. The PFD also indicates the location of every control valve, as control valves play an important role in determining the pressure balance of the process and hence in the sizing of pumps and compressors. A piping and instrumentation diagram (P&ID) is a more detailed version of the PFD that also includes information on ancillary instruments and valves, sampling and drain lines, start-up and shutdown systems, and pipe sizes and metallurgy. The P&ID is used in detailed design and safety analysis.

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This chapter presents an overview of how to read and draw flowsheets and discusses how the unit operations of a process are selected to form the basic process flow structure. Chapter 3 discusses energy flows within a process and describes heat and power recovery methods that are used to make processes more energy-efficient. Chapter 4 covers the use of commercial process simulation tools to generate the heat and material balances for the flowsheet, and Chapter 5 introduces the elements of process control that must be understood to fill in the control systems on the PFD.

2.2 Flowsheet presentation

As the process flowsheet is the definitive document on the process, the presentation must be clear, comprehensive, accurate, and complete. This section describes how to read and draw PFDs.

2.2.1 Block diagrams

A block diagram is the simplest form of flow diagram. Each block can represent a single piece of equipment or a complete stage in the process. Block diagrams are useful for showing simple processes. For complex processes, their use is limited to showing the overall process, broken down into its principal stages.

Block diagrams are useful for representing a process in a simplified form in reports, textbooks, and presentations but have limited use as engineering documents. The stream flow rates and compositions can be shown on the diagram adjacent to the stream lines when only a small amount of information is to be shown or can be tabulated separately.

Fig. 2.1 shows a block flow diagram of a steam reforming process for making hydrogen from methane. The methane feed enters on the left and is mixed with steam and preheated in the convective section of a fired heater. The steam–methane mixture then passes through the reactor tubes in the radiant section of the heater, where the steam reforming reaction takes place:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$

The products from the steam reformer are sent to a shift reactor. The shift reactor increases the amount of hydrogen in the product by allowing the water–gas shift reaction to re-equilibrate at a lower temperature:

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

The shift reactor products are then further cooled and scrubbed in an absorber to remove carbon dioxide before being sent to a pressure-swing adsorption process that separates hydrogen from carbon dioxide, unconverted methane, and water vapor.

Block diagrams are often drawn using simple graphics programs such as Microsoft Visio or PowerPoint. Block flow diagrams are not restricted to using boxes to represent process operations and often use the same flowsheet symbols used in PFDs. Generally, any flowsheet sketch that does not show all the required process equipment should be classified as a block flow diagram.

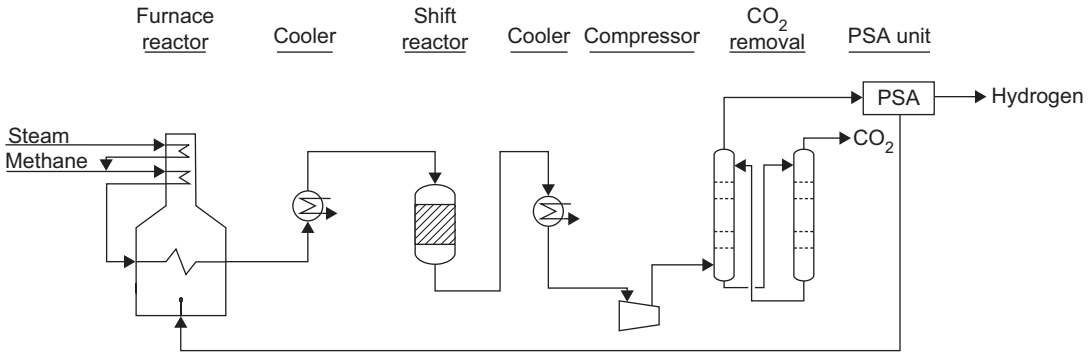


FIG. 2.1 Block flow diagram of steam reforming process for hydrogen.

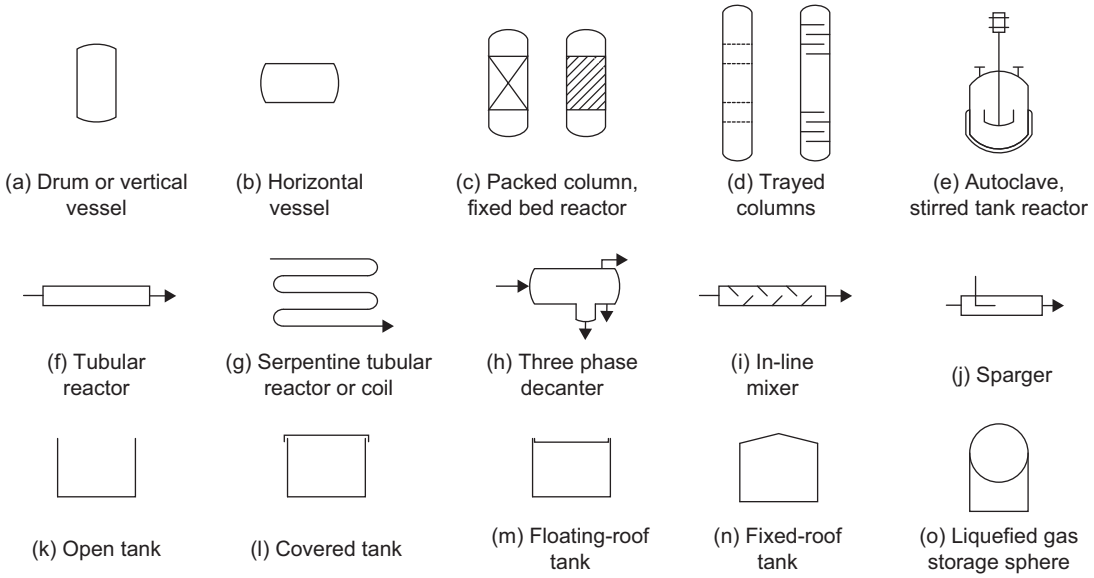


FIG. 2.2 PFD symbols for reactors, vessels, mixers, and tanks

2.2.2 PFD symbols

On the detailed flowsheets used for design and operation, the equipment is normally drawn in a stylized pictorial form. For tender documents or company brochures, actual scale drawings of the equipment are sometimes used, but it is more usual to use a simplified representation. There are several international standards for PFD symbols, but most companies use their own standard symbols, as the cost of converting all of their existing drawings would be excessive. ISO 10628 is the international standard for PFD drawing symbols. Most European countries have adopted ISO 10628 as their standard, but very few North American companies apply this standard, and there is currently no U.S. standard for PFD symbols. The symbols given in British Standard, BS 1553 (1977) "Graphical Symbols for General Engineering" Part 1, "Piping Systems and Plant" are more typical of those in common use. The professional edition of Microsoft Visio contains a library of PFD icons that includes the ISO 10628 symbols, as well as symbols commonly used in the United States and Canada. Examples of standard symbols are given in Appendix A, which is available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

Fig. 2.2 shows symbols that are used for reactors, mixers, vessels, and tanks. Fig. 2.3 shows symbols used for heat transfer equipment. Fig. 2.4 provides symbols for fluid-handling equipment, and Fig. 2.5 gives symbols for solids-handling operations. Some general symbols that are used in combination with other symbols are shown in Fig. 2.6.

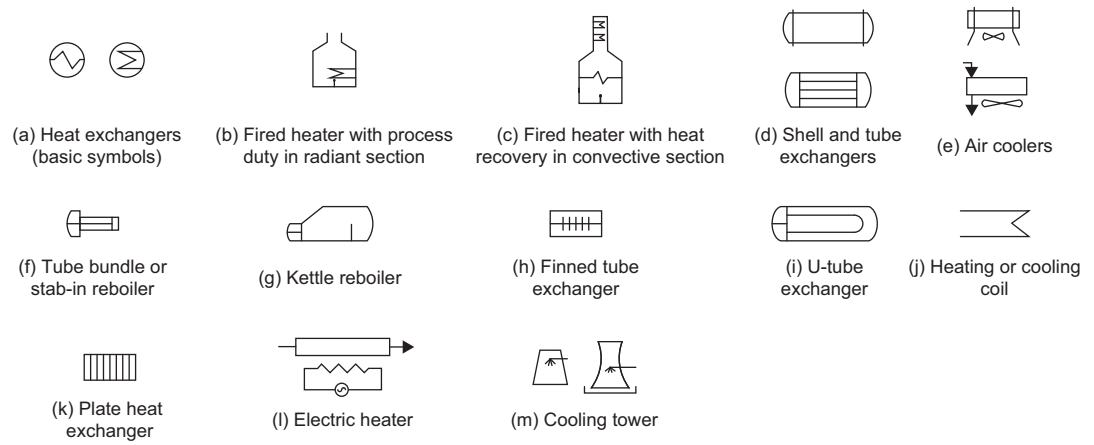


FIG. 2.3 PFD symbols for heat transfer equipment

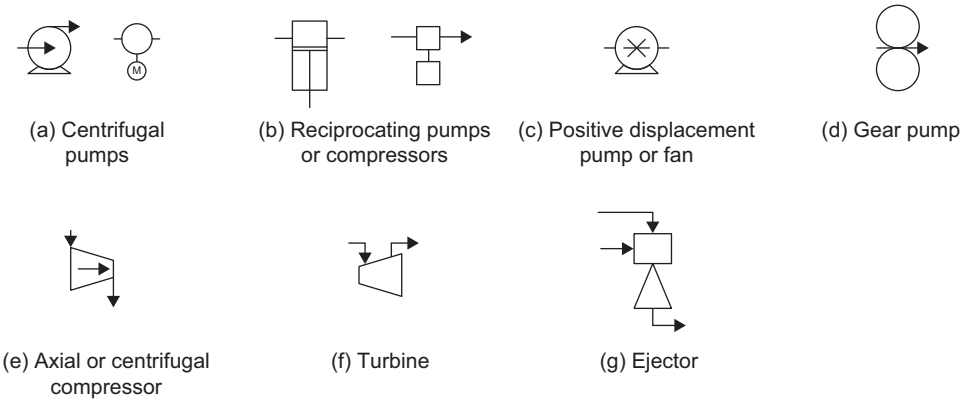


FIG. 2.4 PFD symbols for fluid-handling equipment

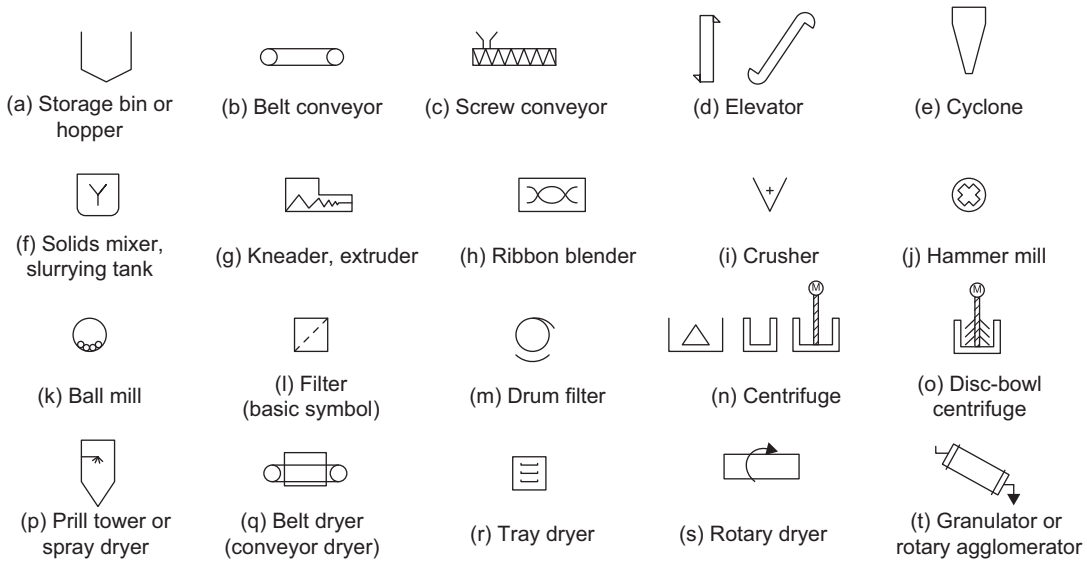


FIG. 2.5 PFD symbols for solids-handling equipment

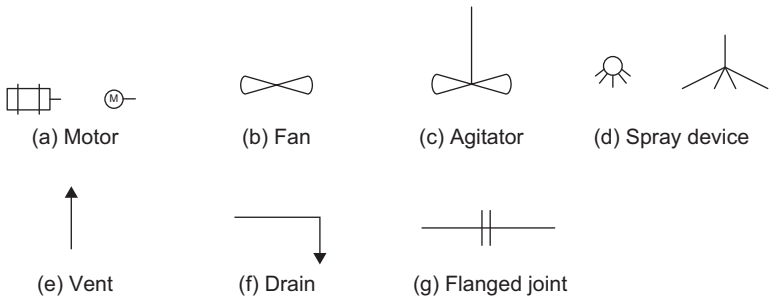


FIG. 2.6 General PFD symbols used with other symbols

The symbols that are used for process instruments, valves, and controllers are given in the section on P&ID diagram symbols in Chapter 5. The operation and design of the different types of equipment illustrated in these figures are described in Part II of this book.

Note that some types of equipment have generic symbols as well as symbols that describe a particular equipment type. If the wrong symbol is selected, this can cause confusion for other engineers who read the flowsheet. For example, Fig. 2.2(*i*) shows an in-line mixer, which would be used downstream of a T-junction to ensure rapid mixing

of two liquid streams. Fig. 2.5(*f*) shows a solids mixer or blender that would be used to mix solids into a liquid. Fig. 2.6(*c*) is the symbol for a propeller agitator that might be used in a mixing tank. All of these symbols could be referred to as a *mixer*, but the designer's intention is obviously different in each case. Some abbreviations that are commonly used in PFDs are listed in the nomenclature at the end of this chapter.

2.2.3 Presentation of stream flow rates

The data on the flow rate of each individual component, on the total stream flow rate, and the percentage composition can be shown on the flowsheet in various ways. The simplest method, suitable for simple processes with few pieces of equipment, is to tabulate the data in blocks alongside the process stream lines, as shown in Fig. 2.7. Only a limited amount of information can be shown this way, and it is difficult to make neat alterations or to add more data.

A better method for the presentation of data on flowsheets is shown in Figs. 2.8 and 2.9. In this method each stream line is numbered and the data are tabulated at the bottom of the sheet. Alterations and additions can be easily made. This is the method generally used by professional design offices. A typical commercial flowsheet is shown in Fig. 2.10. Guide rules for the layout of this type of flowsheet presentation are given in Section 2.2.5.

2.2.4 Information to be included

The amount of information shown on a flowsheet will depend on the custom and practice of the particular design office. The list given here has therefore been divided into essential items and optional items. The essential items must always be shown; the optional items add to the usefulness of the flowsheet but are not always included.

Essential information

1. Always show *all* process equipment, including feed and product storage and equipment used for transporting fluids and solids.
2. Always indicate the location of process control valves.
3. For stream composition, either:
   - i. Tabulate the flow rate of each individual component, kg/h, which is preferred,
   - ii. Or give the stream composition as a weight fraction.
4. Total stream flow rate, kg/h.
5. Stream temperature, degrees Celsius preferred.
6. Nominal operating pressure (the required operating pressure).

Optional information

1. Molar percentage composition and/or molar flow rates.
2. Stream enthalpy, kJ/h.
3. Physical property data, with mean values for the stream, such as:
   - i. Density, kg/m^3
   - ii. Viscosity, $mN\ s/m^2$
4. Stream name: a brief one- or two-word description of the nature of the stream, for example, "ACETONE COLUMN BOTTOMS"

The convention of showing control valves on a PFD is not followed by all companies, but is recommended as a best practice. The presence of a control valve always causes pressure drop and may create a requirement for additional pumps or compressors. Showing the control valves can help identify locations where the designer may have overlooked the need for a pump.

Effective cooperation depends on effective communications, and all design organizations have formal procedures for handling project information and documentation. The project documentation will include:

1. General correspondence within the design group and with:
   - i. government departments
   - ii. equipment vendors
   - iii. site personnel
   - iv. the client

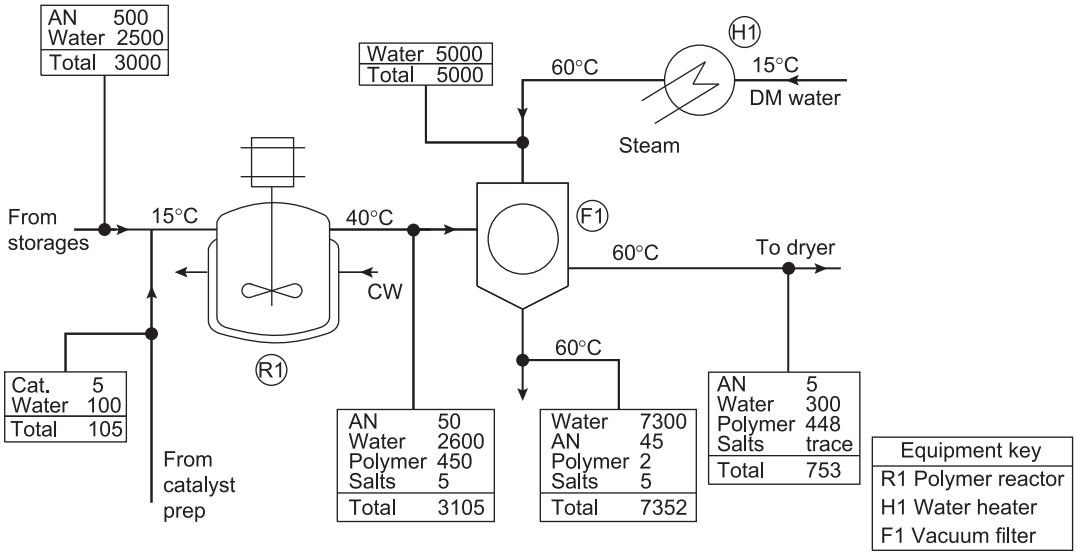


FIG. 2.7 Flowsheet: Polymer production.

2. Calculation sheets:
- **i.** design calculations
- **ii.** cost estimates
- **iii.** material and energy balances

3. Drawings:
- **i.** flow sheets
- **ii.** piping and instrumentation diagrams
- **iii.** layout diagrams
- **iv.** plot/site plans
- **v.** equipment details
- **vi.** piping diagrams (isometrics)
- **vii.** architectural drawings
- **viii.** design sketches

4. Specification sheets:
- **i.** the design basis
- **ii.** feed and product specifications
- **iii.** an equipment list
- **iv.** sheets for equipment, such as heat exchangers, pumps, heaters, etc.

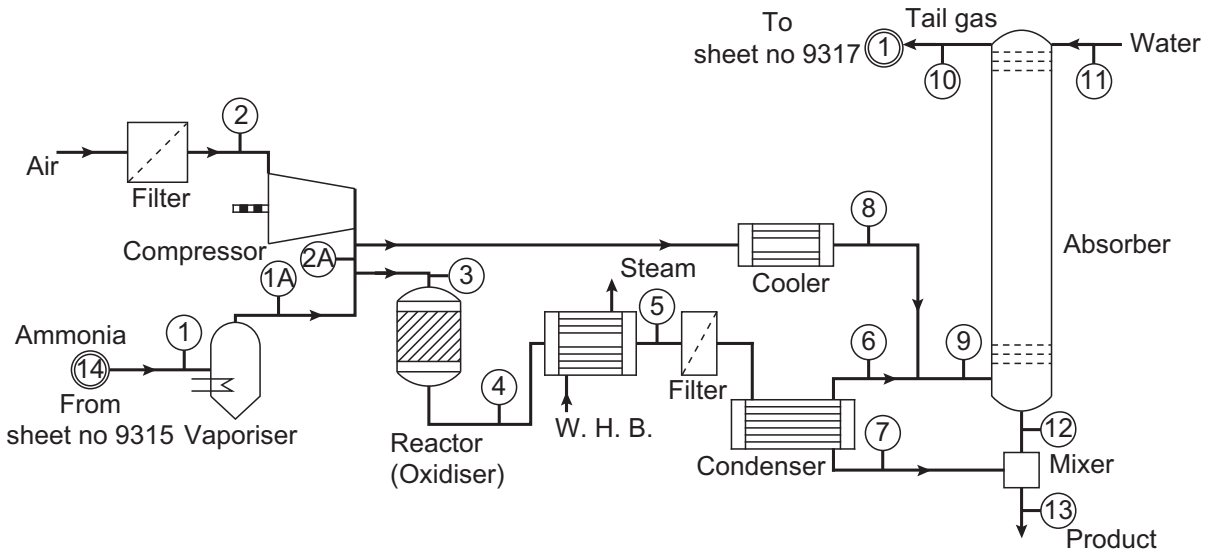
5. Health, safety, and environmental information:
- **i.** materials safety data sheets (MSDS forms)
- **ii.** HAZOP or HAZAN documentation (see Chapter 10)
- **iii.** emissions assessments and permits

5. Purchase orders:
- **i.** quotations
- **ii.** invoices

All documents are assigned a code number for easy cross-referencing, filing, and retrieval.

2.2.5 Layout

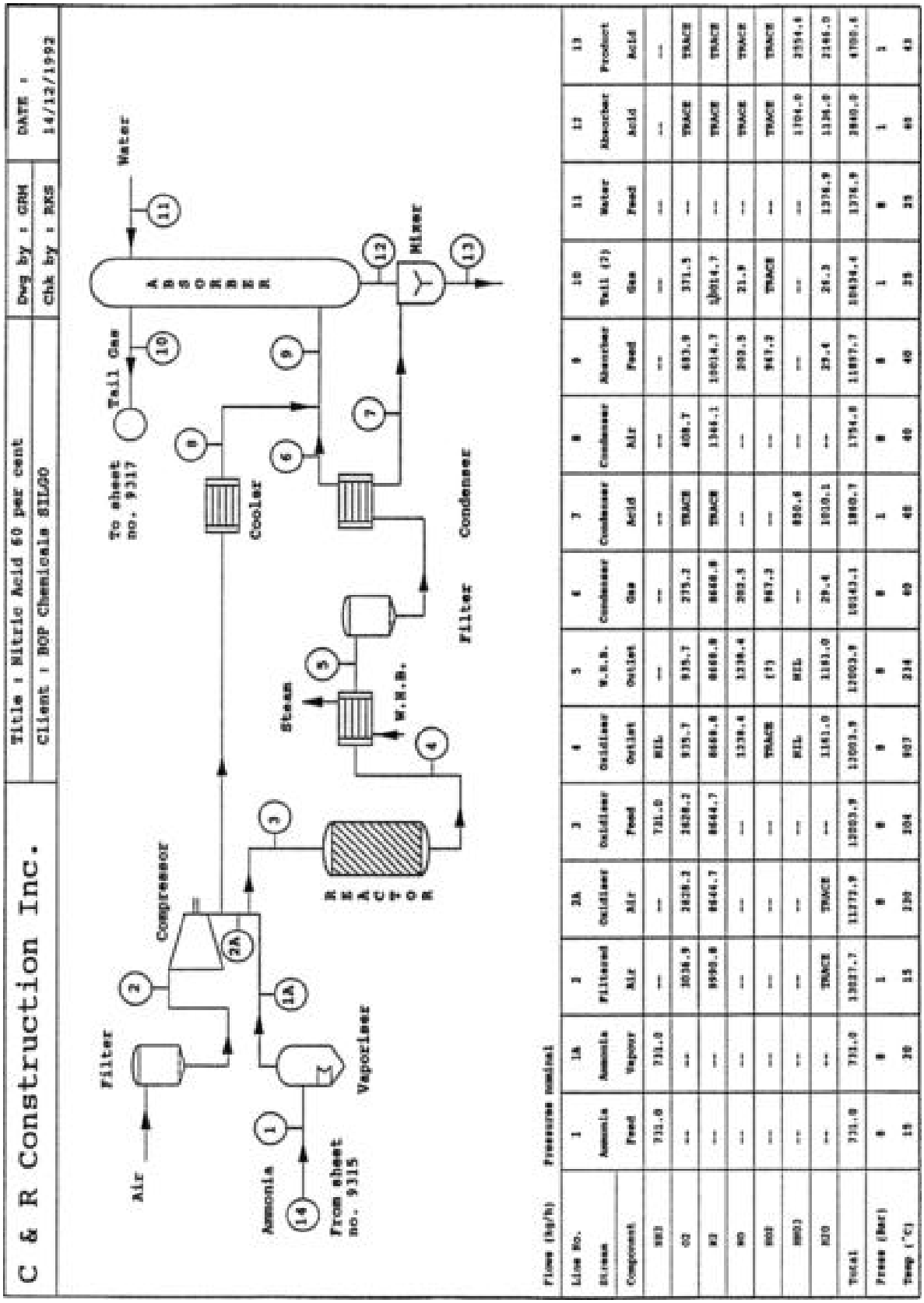
The sequence of the main equipment items shown symbolically on the flowsheet follows that of the proposed plant layout. Some license must be exercised in the placing of ancillary items, such as heat exchangers and pumps, or the layout will be too congested. The aim should be to show the flow of material from stage to stage as it will occur and to give a general impression of the layout of the actual process plant.



Flows kg/h pressures nominal

Line no. / Stream component	1 Ammonia feed	1A Ammonia vapor	2 Filtered air	2A Oxidiser air	3 Oxidiser feed	4 Oxidiser outlet	5 W.H.B. outlet	6 Condenser gas	7 Condenser acid	8 Secondary air	9 Absorber feed	10 Tail(2) gas	11 Water feed	12 Absorber acid	13 Product acid	C & R Construction Inc
NH_3	731.0	731.0	—	—	731.0	Nil	—	—	—	—	—	—	—	—	—	Nitric acid 60 percent
O_2	—	—	3036.9	2628.2	2628.2	935.7	(935.7)(1)	275.2	Trace	408.7	683.9	371.5	—	Trace	Trace	100,000 t/y
N_2	—	—	9990.8	8644.7	8644.7	8668.8	8668.8	8668.8	Trace	1346.1	10,014.7	10,014.7	—	Trace	Trace	Client BOP chemicals
NO	—	—	—	—	—	1238.4	(1238.4)(1)	202.5	—	—	202.5	21.9	—	Trace	Trace	SLIGO
NO_2	—	—	—	—	—	Trace	(?)(1)	967.2	—	—	967.2	(Trace)(1)	—	Trace	Trace	Sheet no. 9316
HNO_3	—	—	—	—	—	Nil	Nil	—	850.6	—	—	—	—	1704.0	2554.6	
H_2O	—	—	Trace	—	—	1161.0	1161.0	29.4	1010.1	—	29.4	26.3	1376.9	1136.0	2146.0	
Total	731.0	731.0	13,027.7	11,272.9	12,003.9	12,003.9	12,003.9	10,143.1	1860.7	1754.8	11,897.7	10,434.4	1376.9	2840.0	4700.6	
Press bar	8	8	1	8	8	8	8	8	1	8	8	1	8	1	1	Dwg by Date
Temp. °C	15	20	15	230	204	907	234	40	40	40	40	25	25	40	43	Checked 25/7/1980

FIG. 2.8 Flowsheet: Simplified nitric acid process.



Flows (kg/h)	Pressures nominal																	
Line No.	1	1A	2	2A	3	4	5	6	7	8	9	10	11	12	13
Stream	Ammonia Feed	Ammonia Vapour	Filtered Air	Oxidiser Air	Oxidiser Feed	Oxidiser Outlet	W.H.B. Outlet	Condenser Gas	Condenser Acid	Condenser Air	Absorber Feed	Tail (T) Gas	Water Feed	Absorber Acid	Product Acid
Component															
NH3	731.0	731.0	---	---	731.0	815	---	---	---	---	---	---	---	---	---
O2	--	--	3038.3	2428.3	2428.3	815.7	815.7	215.2	TRACE	408.7	623.9	371.5	---	TRACE	TRACE
N2	---	---	9995.8	8444.7	8444.7	8888.8	8888.8	8888.8	TRACE	1568.1	10014.7	10014.7	---	TRACE	TRACE
H2O	---	---	---	---	---	1238.4	1238.4	282.5	---	---	282.5	31.9	---	TRACE	TRACE
HNO3	---	---	---	---	---	TRACE	(T)	957.2	---	---	957.2	TRACE	---	TRACE	TRACE
HNO3	---	---	---	---	---	815	815	---	850.8	---	---	---	---	1704.9	2554.4
H2O	---	---	TRACE	TRACE	---	1181.0	1181.0	28.4	1810.1	---	28.4	28.2	1376.9	1136.8	2186.0
Total	731.0	731.0	13037.7	11272.9	12003.9	13003.9	13003.9	10440.1	1660.7	1754.8	11887.7	10454.4	1376.9	2840.8	4740.4
Press (Bar)	6	6	1	6	6	6	6	6	1	6	6	1	6	1	1
Temp (°C)	15	30	15	150	304	907	334	40	40	40	40	35	35	40	40

FIG. 2.9 Alternative presentation.

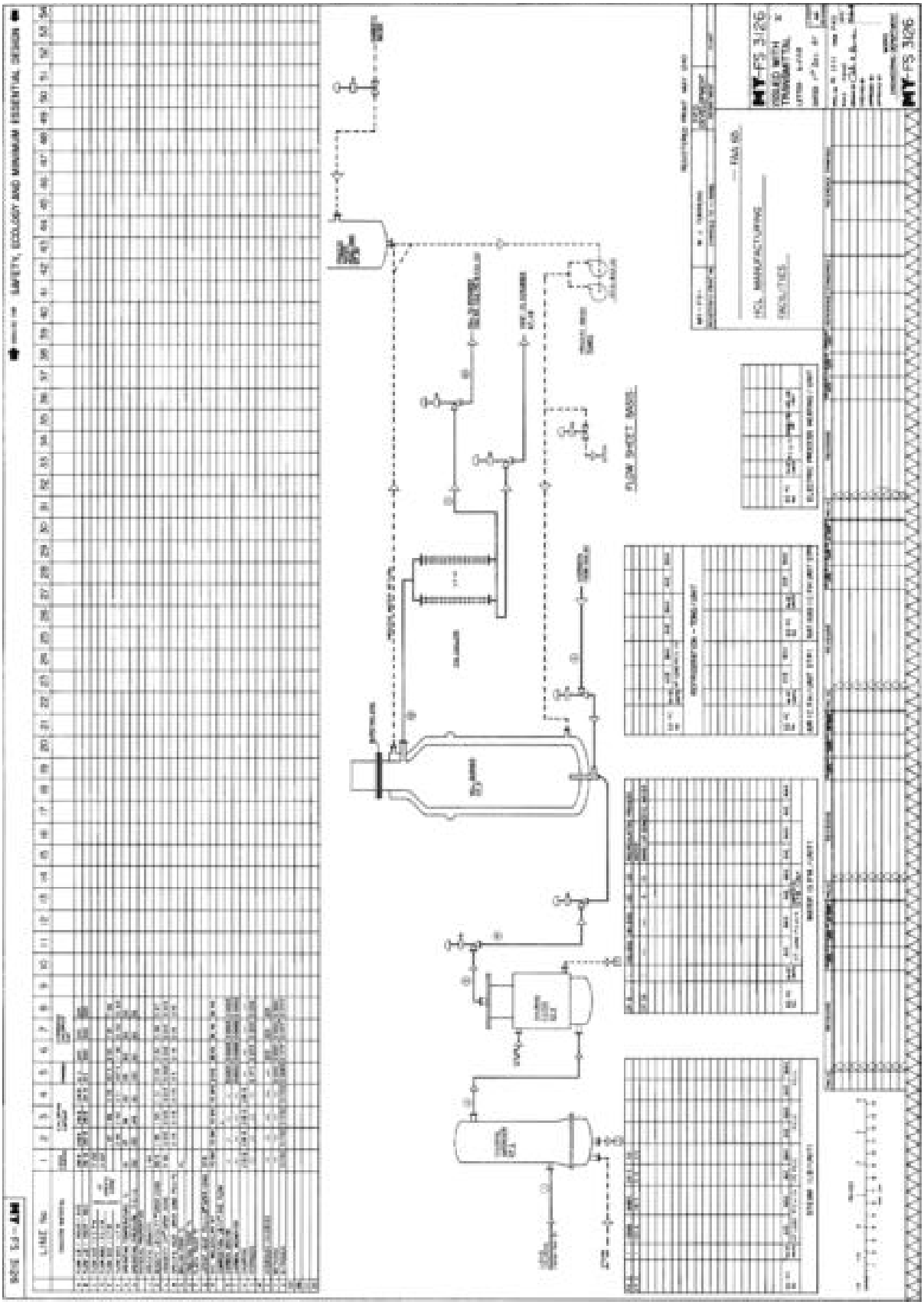


FIG. 2.10 A typical flowsheet.

The equipment should be drawn approximately to scale. Again, some license is allowed for the sake of clarity, but the principal equipment items, such as reactors, vessels, and columns, should be drawn roughly in the correct proportion. Ancillary items can be drawn out of proportion. For a complex process with many process units, several sheets may be needed, and the continuation of the process streams from one sheet to another must be clearly shown. One method of indicating a line continuation is shown in Fig. 2.8; those lines that are continued over to another drawing are indicated by a double concentric circle around the line number, and the continuation sheet number is written below. An alternative method is to extend lines to the side of the page and then indicate the drawing sheet on which the line is continued.

The overall process flow will usually be from left to right across the diagram, with recycle streams flowing right to left. Streams should be shown entering and leaving vessels in a manner that is consistent with the stream phase, density, and mode of operation. When a vessel has multiple feeds or products, their arrangement in the diagram should correspond to the physical arrangement intended by the designer. For example, the gas feed to an absorption column should enter below the bottom tray, the liquid feed should enter on the top tray, gas product should be shown leaving the top of the vessel, and liquid product should be shown leaving the bottom of the vessel.

The equipment should be well spaced out so that streams can be labeled without the drawing becoming cluttered. It is better to use several continuation sheets than to try to fit everything on one page.

The table of stream flows and other data can be placed above or below the equipment layout. Normal practice is to place it below. The components should be listed down the left side of the table, as in Figs. 2.8 and 2.9. For a long table, it is good practice to repeat the list at the right side so the components can be traced across from either side.

The stream line numbers should follow consecutively from left to right of the layout as far as is practicable, so that when reading the flowsheet it is easy to locate a particular line and the associated column containing the data.

All the process stream lines shown on the flowsheet should be numbered and the data for the stream given. On a large flowsheet, the designers sometimes use different series of numbers for different plant sections; for example, beginning the stream numbering at 100 for feed preparation, 200 for reaction, 300 for separation, and 400 for purification. This can be helpful in quickly tracing a stream to a section of the plant. There is always a temptation to leave out the data on a process stream if it is clearly just formed by the addition of two other streams, as at a junction, or if the composition is unchanged when flowing through a process unit, such as a heat exchanger; this temptation should be avoided. What may be clear to the process designer is not necessarily clear to the others who will use the flowsheet. Complete, unambiguous information on all streams should be given, even if this involves some repetition. The purpose of the flowsheet is to show the function of each process unit, even when the function has no discernible impact on the mass and energy balance.

2.2.6 Precision of data

The total stream and individual component flows do not normally need to be shown to a high precision on the process flowsheet; three or four significant figures are all that is usually justified by the accuracy of the flowsheet calculations and will typically be sufficient. The flows should, however, balance to within the precision shown. If a stream or component flow is so small that it is less than the precision used for the larger flows, it can be shown to a greater number of places if its accuracy justifies this and the information is required. If the composition of a component is very low but is specified as a process constraint, as, say, for an effluent stream or product quality specification, it can be shown in parts per million (ppm). Imprecise small flows are best shown as "TRACE."

A trace quantity should not be shown as zero, nor should the space in the tabulation be left blank, unless the process designer *is sure* that it has no significance. The process designer should be aware that if the space in the data table is left blank opposite a particular component, the quantity may be assumed to be zero by the specialist design groups, who take their information from the flowsheet. Trace quantities can be important. Only a trace of an impurity is needed to poison a catalyst, and trace quantities can determine the selection of the materials of construction; see Chapter 6.

2.2.7 Basis of the calculation

It is good practice to show on the flowsheet the basis used for the flowsheet calculations. This includes the operating hours per year, the reaction and physical yields, and the datum temperature used for energy balances. It is also helpful to include a list of the principal assumptions used in the calculations. This alerts the user to any limitations that may have to be placed on the flowsheet information.

If the amount of information that needs to be presented is excessive, it can be summarized in a separate document that is referenced on the flowsheet.

In some cases, mass and energy balances are prepared for multiple scenarios. These might include winter and summer operating conditions, start of catalyst life and end of catalyst life, manufacture of different products or product grades, etc. Usually these different scenarios are shown as several tables on the same flowsheet, but occasionally different flowsheets are drawn for each case.

2.2.8 Batch processes

Flowsheets drawn up for batch processes normally show the quantities required to produce one batch. If a batch process forms part of an otherwise continuous process, it can be shown on the same flowsheet, providing a clear break is made when tabulating the data between the continuous and batch sections (i.e., the change from kg/h to kg/batch).

A continuous process may include batch make-up of minor reagents, such as the catalyst for a polymerization process. Batch flows into a continuous process are usually labeled "Normally no flow" and show the flow rates that will be obtained when the stream is flowing. It is these instantaneous flow rates that govern the equipment design rather than the much lower time-averaged flow rates.

2.2.9 Utilities

To avoid cluttering up the flowsheet, it is not normal practice to show the utility (service) headers and lines on the process flowsheet. The utility connections required on each piece of equipment should be shown and labeled, for example, "CTW" for cooling tower water. The utility requirements for each piece of equipment should be tabulated on the flowsheet. A glossary of common abbreviations used for utility streams in PFDs is given in the nomenclature at the end of this chapter. Utility systems are described in more detail in Chapter 3.

2.2.10 Equipment identification

Each piece of equipment shown on the flowsheet must be identified with a code number and name. The identification number (usually a letter and some digits) is normally that assigned to a particular piece of equipment as part of the general project control procedures and is used to identify it in all the project documents.

If the flowsheet is not part of the documentation for a project, then a simple, but consistent, identification code should be devised. The easiest code is to use an initial letter to identify the type of equipment, followed by digits to identify the particular piece. For example, H — heat exchangers, C — columns, R — reactors. Most companies have a standard convention that should be followed, but if there is no agreed standard, then the key to the code should be shown on the flowsheet.

2.2.11 Flowsheet drafting programs

Most design offices use drafting software for the preparation of flowsheets and other process drawings. With drafting software, standard symbols representing the process equipment, instruments, and control systems are held in files, and these symbols are called up as required when drawing flowsheets and piping and instrumentation diagrams. Final flowsheet drawings are usually produced by professional drafters, who are experienced with the drafting software and conventions, rather than by the design engineer. The design engineer has to provide the required numbers, sketch the flowsheet, and review the final result.

Although most process simulation programs feature a graphical user interface (GUI) that creates a drawing that resembles a PFD, printouts of these drawings should not be used as actual PFDs. The unit operations shown in the process simulation usually do not exactly match the unit operations of the process. The simulation may include dummy items that do not physically exist and may omit some equipment that is needed in the plant but is not part of the simulation.

2.3 The anatomy of a chemical manufacturing process

This section describes the basic components of chemical processes and discusses how designers select between batch and continuous processes. The effects of reactor yield and selectivity on flowsheet structure are examined and used to illustrate how flowsheets become complex when there are multiple feeds and products.

2.3.1 Components of a chemical process

The basic components of a typical chemical process are shown in Fig. 2.11, in which each block represents a stage in the overall process for producing a product from the raw materials. Fig. 2.11 represents a generalized process; not all the stages will be needed for any particular process, and the complexity of each stage will depend on the nature of the process. Chemical engineering design is concerned with the selection and arrangement of the stages and the selection, specification, and design of the equipment required to perform the function of each stage.

Stage 1. Raw material storage

Unless the raw materials (also called *feed stocks* or *feeds*) are supplied as intermediate products (intermediates) from a neighboring plant, some provision will have to be made to hold several days', or weeks', worth of storage to smooth out fluctuations and interruptions in supply. Even when the materials come from an adjacent plant, some provision is usually made to hold inventory for a few hours, or even days, to decouple the processes. The storage required depends on the nature of the raw materials, the method of delivery, and what assurance can be placed on the continuity of supply. If materials are delivered by ship (tanker or bulk carrier) several weeks' worth of stocks may be necessary, whereas if they are received by road or rail in smaller lots, less storage will be needed.

Stage 2. Feed preparation

Some purification and preparation of the raw materials will usually be necessary before they are sufficiently pure, or in the right form, to be fed to the reaction stage. For example, acetylene generated by the carbide process contains arsenic and sulfur compounds and other impurities, which must be removed by scrubbing with concentrated sulfuric acid (or other processes) before it is sufficiently pure for reaction with hydrochloric acid to produce dichloroethane. Feed contaminants that can poison process catalysts, enzymes, or microorganisms must be removed. Liquid feeds need to be vaporized before being fed to gas- phase reactors, and solids may need crushing, grinding, and screening. Solid feeds may also need to be weighed and mixed into slurries or solutions so that they can be brought to process pressure and easily mixed with other components.

The feed preparation stage always includes means for getting the feeds out of storage and into the process. Liquids are usually pumped out of storage through control valves that regulate the feed flow rate. Gases and vapors may need compression if the storage is not pressurized. Solids are conveyed from storage using a variety of equipment, described in Chapter 18.

Biological processes require careful feed preparation. The growth media and any other fluids that are fed to the cell culture must be sterile to prevent unwanted organisms from entering the process. Sterilization is usually accomplished by heating the feed to a high temperature and keeping it hot for long enough to kill unwanted organisms, then cooling the feed to the desired temperature for the reactor. The preparation of biological reactor feeds is discussed in more detail in Section 15.9.

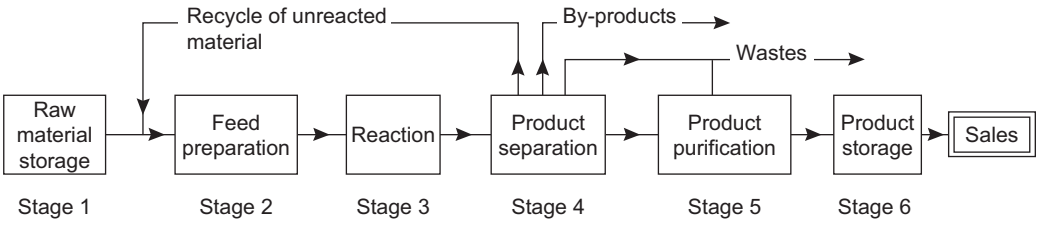


FIG. 2.11 Anatomy of a chemical process.

Stage 3. Reaction

The reaction stage is the heart of a chemical manufacturing process. In the reactor the raw materials are brought together under conditions that promote the production of the desired product; almost invariably, some by-products will also be formed, either through the reaction stoichiometry, by side reactions, or from reactions of impurities present in the feed. Reactor design is discussed in Chapter 15.

Stage 4. Product separation

After the reactor(s), the products and by-products are separated from any unreacted material. If in sufficient quantity, the unreacted material will be recycled to the reaction stage or to the feed purification and preparation stage. The by-products may also be separated from the products at this stage and may undergo further processing for recovery or sale. In most chemical processes there are multiple reaction steps, each followed by one or more separation steps.

Stage 5. Purification

Before sale, the main product will often need purification to meet the product specifications. If produced in economic quantities, the by-products may also be purified for sale. For by-products, there will always be an economic trade-off between purifying the by-product for sale or disposing of it as recycle or waste.

Stage 6. Product storage

Some inventory of finished product must be held to match production with sales. Provision for product packaging and transport is also needed, depending on the nature of the product. Liquids are normally dispatched in drums and in bulk tankers (road, rail, and sea); solids in sacks, cartons, or bales.

The amount of stock that is held will depend on the nature of the product and the market.

Ancillary processes

In addition to the main process stages shown in Fig. 2.11, provision must be made for the supply of the utilities needed, such as process water, cooling water, compressed air, and steam. The design of utility systems is discussed in Chapter 3.

2.3.2 Continuous and batch processes

Continuous processes are designed to operate 24 hours a day, 7 days a week, throughout the year. Some downtime will be allowed for maintenance and, in some processes, for catalyst regeneration. The plant attainment or operating rate is the percentage of the available hours in a year that the plant operates and is usually between 90% and 95%.

$$\text{Attainment } \% = \frac{\text{hours operated}}{8760} \times 100 \tag{2.1}$$

A typical design basis would assume 8000 operating hours per year.

Batch processes are designed to operate intermittently, with some, or all, of the process units being frequently shut down and started up. It is quite common for batch plants to use a combination of batch and continuous operations. For example, a batch reactor may be used to feed a continuous distillation column.

Continuous processes will usually be more economical for large-scale production. Batch processes are used when some flexibility is wanted in production rate or product specifications.

The advantages of batch processing are:

- Batch processing allows production of multiple different products or different product grades in the same equipment.
- In a batch plant, the integrity of a batch can be preserved as it moves from operation to operation. This can be useful for quality control purposes.
- The production rate of batch plants is flexible, as there are no turn-down issues when operating at low output.
- Batch plants are easier to clean and maintain sterile operation.
- Batch processes are easier to scale up from chemist's recipes.
- Batch plants have low capital for small production volumes. The same piece of equipment can often be used for several unit operations.

The drawbacks of batch processing are:

- The scale of production is limited.
- It is difficult to achieve economies of scale by going to high production rates.
- Batch-to-batch quality can vary, leading to high production of waste products or off-spec product.
- Recycle and heat recovery are harder, making batch plants less energy efficient and more likely to produce waste by-products.
- Asset utilization is lower for batch plants, as the plant almost inevitably is idle part of the time.
- Batch plants are more labor-intensive, and so the fixed costs of production are much higher for batch plants on a $/unit mass of product basis.

Choice of continuous versus batch production

Given the higher fixed costs and lower plant utilization of batch processes, batch processing usually only makes sense for products that have high value and are produced in small quantities. Batch plants are commonly used for:

- Food products
- Pharmaceutical products such as drugs, vaccines, and hormones
- Personal care products
- Blended products with multiple grades, such as paints, detergents, etc.
- Specialty chemicals

Even in these sectors, continuous production is favored if the process is well understood, the production volume is large, and the market is competitive.

2.3.3 Effect of reactor conversion and yield on flowsheet structure

It is important to distinguish between conversion and yield. Conversion has to do with reactants; yield with products.

Conversion

Conversion is a measure of the fraction of the reagent that reacts. To optimize reactor design and minimize by-product formation, the conversion of a particular reagent is often less than 100%. If more than one reactant is used, the reagent on which the conversion is based must be specified.

Conversion is defined by the following expression:

$$\begin{aligned}\text{Conversion} &= \frac{\text{amount of reagent consumed}}{\text{amount supplied}} \\ &= \frac{(\text{amount in feed stream}) - (\text{amount in product stream})}{(\text{amount in feed stream})}\end{aligned} \tag{2.2}$$

This definition gives the total conversion of the particular reagent to all products.

Example 2.1

In the manufacture of vinyl chloride (VC) by the pyrolysis of dichloroethane (DCE), the reactor conversion is limited to 55% to reduce carbon formation, which fouls the reactor tubes.

Calculate the quantity of DCE fed to the reactor to produce 5000 kg/h VC.

Solution

Basis: 5000 kg/h VC (the required quantity).

$$\text{Reaction: } C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl$$

Molar weights: DCE 99, VC 62.5

$$\text{kmol/h VC produced} = \frac{5000}{62.5} = \underline{\underline{80}}$$

From the stoichiometric equation, 1 kmol DCE produces 1 kmol VC. Let X be DCE feed in kmol/h:

$$\text{Percent conversion} = 55 = \frac{80}{X} \times 100$$

$$X = \frac{80}{0.55} = \underline{\underline{145.5 \text{ kmol/h}}}$$

In this example, the small loss of DCE to carbon and other products has been neglected. All the DCE reacted has been assumed to be converted to VC.

Selectivity

Selectivity is a measure of the efficiency of the reactor in converting reagent to the desired product. It is the fraction of the reacted material that was converted into the desired product. If no by-products are formed, then the selectivity is 100%. If side reactions occur and by-products are formed, then the selectivity decreases. Selectivity is always expressed as the selectivity of feed A for product B and is defined by the equation:

$$\text{Selectivity} = \frac{\text{moles of B formed}}{\text{moles of B that could have been formed if all A reacted to give B}}$$

$$= \frac{\text{moles of B formed}}{\text{moles of A consumed} \times \text{stoichiometric factor}} \tag{2.3}$$

$$\text{Stoichiometric factor} = \text{moles of B produced per mole of A reacted in the reaction stoichiometric equation}$$

Selectivity is usually improved by operating the reactor at low conversion. At high conversion, the reactor has low concentrations of at least one reagent and high concentrations of products, so reactions that form by-products are more likely to occur.

Reagents that are not converted in the reactor can be recovered and recycled. Reagents that become converted to by-products usually cannot be recovered, and the by-products must be purified for sale or else disposed as waste (see Section 8.2.3). The optimum reactor conditions thus usually favor low reactor conversion to give high selectivity for the desired products when all of these costs are taken into account.

Yield

Yield is a measure of the performance of a reactor or plant. Several different definitions of yield are used, and it is important to clearly state the basis of any yield numbers. This is often not done when yields are quoted in the literature, and judgment must be used to decide what was intended.

The yield of product B from feed A is defined by:

$$\text{Yield} = \frac{\text{moles of B formed}}{\text{moles of A supplied} \times \text{stoichiometric factor}} \tag{2.4}$$

For a reactor, the yield is the product of conversion and selectivity:

$$\text{Reaction yield} = \text{Conversion} \times \text{Selectivity}$$

$$= \frac{\text{moles A consumed}}{\text{moles A supplied}} \times \frac{\text{moles B formed}}{\text{moles A consumed} \times \text{stoichiometric factor}} \tag{2.5}$$

With industrial reactors, it is necessary to distinguish between "reaction yield" (chemical yield), which includes only chemical losses to side products, and the overall "reactor yield," which also includes physical losses, such as losses by evaporation into vent gas.

If the conversion is near 100% it may not be worth separating and recycling the unreacted material; the overall process yield would then include the loss of unreacted material. If the unreacted material is separated and recycled, the overall process yield *taken over the reactor and separation step* would include any physical losses from the separation step.

Plant yield is a measure of the overall performance of the plant and includes all chemical and physical losses.

Plant yield (applied to the complete plant or any stage):

$$= \frac{\text{moles of product produced}}{\text{moles of reagent supplied to the process} \times \text{stoichiometric factor}} \tag{2.6}$$

Where more than one reagent is used or product produced, it is essential that the product and reagent to which the yield refers are clearly stated.

The plant yield of B from A is the product of the reactor selectivity of feed A for product B and the separation efficiency (recovery) of each separation step that handles product B or reagent A. As a useful check, the plant yield should be greater than the reactor yield if a separation and feed recycle scheme has been implemented. If the feed recovery and recycle system were 100% efficient, the plant yield would approach the reactor selectivity.

Example 2.2

In the production of ethanol by the hydrolysis of ethylene, diethyl ether is produced as a by-product. A typical feed stream composition is 55% ethylene, 5% inerts, 40% water, and product stream: 52.26% ethylene, 5.49% ethanol, 0.16% ether, 36.81% water, and 5.28% inerts. Calculate the selectivity of ethylene for ethanol and for ether.

Solution

$$\text{Reactions: } C_2H_4 + H_2O \rightarrow C_2H_5OH$$

$$2C_2H_5OH \rightarrow (C_2H_5)_2O + H_2O$$

Basis: 100 moles feed (easier calculation than using the product stream)

Note: The flow of inerts will be constant, as they do not react, and it can thus be used to calculate the other flows from the compositions.

Feed stream

ethylene	55 mol
inerts	5 mol
water	40 mol

Product stream

$$\text{ethylene} = \frac{52.26}{5.28} \times 5 = 49.49 \text{ mol}$$

$$\text{ethanol} = \frac{5.49}{5.28} \times 5 = 5.20 \text{ mol}$$

$$\text{ether} = \frac{0.16}{5.28} \times 5 = 0.15 \text{ mol}$$

$$\text{Amount of ethylene reacted}: = 55.0 - 49.49 = 5.51 \text{ mol}$$

$$\text{Selectivity of ethylene for ethanol}: = \frac{5.20}{5.51 \times 1.0} \times 100 = \underline{\underline{94.4\%}}$$

As 1 mol of ethanol is produced per mol of ethylene, the stoichiometric factor is 1.

$$\text{Selectivity of ethylene for ether}: = \frac{0.15}{5.51 \times 0.5} \times 100 = \underline{\underline{5.44\%}}$$

The stoichiometric factor is 0.5, as 2 mol of ethylene produce 1 mol of ether.

Note that the conversion of ethylene to all products is given by:

$$\text{Conversion} = \frac{\text{mols fed} - \text{mols out}}{\text{mols fed}} = \frac{55 - 49.49}{55} \times 100$$

$$= \underline{\underline{10 \text{ percent}}}$$

The selectivity based on water could also be calculated but is of no real interest, as water is relatively inexpensive compared with ethylene. Water is clearly fed to the reactor in considerable excess.

The yield of ethanol based on ethylene is:

$$\text{Reaction yield} = \frac{5.20}{55 \times 1.0} \times 100 = \underline{\underline{9.45\%}}$$

Example 2.3

In the chlorination of ethylene to produce DCE, the conversion of ethylene is reported as 99.0%. If 94 mol of DCE are produced per 100 mol of ethylene reacted, calculate the selectivity and the overall yield based on ethylene. The unreacted ethylene is not recovered.

Solution

$$\text{Reaction: } C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$$

The stoichiometric factor is 1.

$$\text{Selectivity} = \frac{\text{moles DCE produced}}{\text{moles ethylene reacted} \times 1} \times 100$$

$$= \frac{94}{100} \times 100 = \underline{\underline{94\%}}$$

$$\text{Overall yield (including physical losses)} = \frac{\text{moles DCE produced}}{\text{moles ethylene fed} \times 1} \times 100$$

Ninety-nine moles of ethylene are reacted for 100 moles fed, so

$$\text{Overall yield} = \frac{94}{100} \times \frac{99}{100} = \underline{\underline{93.1\%}}$$

Note that we get the same answer by multiplying the selectivity (0.94) and conversion (0.99).
The principal by-product of this process is trichloroethane.

Effect of conversion, selectivity, and yield on flowsheet structure

Very few processes produce the desired product in stoichiometric yield with no by-products and no equilibrium limitations.

If the desired reaction is limited by equilibrium between the feeds and products, the reaction will not proceed to 100% conversion in the reactor, and it will be necessary to separate the product from unreacted feed components. It will usually be economically attractive to recover the unconverted feeds either to the reactor section or to the feed preparation section of the plant.

In most chemical processes the designer must also address the formation of by-products through unwanted reactions, in which case the selectivity of the feed for the desired product is less than 100%. The presence of nonselective reactions can have a number of undesirable effects on process economics. The most important impact of by-product formation is that by-products represent a loss of potential product. Because feedstock costs are usually the main component of the overall cost of production, low selectivity can have a strong negative impact on process economics. The by-products must be separated from the desired product, causing additional complexity and cost in the separation section. If the by-products have value, they can be purified and sold, but this adds more equipment to the process. If the by-products are not worth recovering, then in some cases they can be recycled within the process and converted back to feed or products. These recycles also add cost and complexity to the process. If the by-products cannot be sold or recycled, they must be disposed of as waste streams. Additional processing steps may be needed to bring the waste stream to a safe condition for discharge or disposal.

Because of the high costs of dealing with by-products, most processes are operated under conditions that maximize reactor selectivity. This often means operating at low conversion and accepting large recycles of feeds. Alternatively, a cheaper feed may be used in excess, so that a high conversion of the more expensive feed can be achieved at high selectivity, as discussed in the following section.

Use of excess reagent

In industrial reactions the components are seldom fed to the reactor in exact stoichiometric proportions. A reagent may be supplied in excess to promote the desired reaction; to maximize the use of an expensive reagent; or to ensure complete reaction of a reagent, as in combustion.

The percentage excess reagent is defined by the following equation:

$$\text{Percent excess} = \frac{\text{quantity supplied} - \text{stoichiometric}}{\text{stoichiometric quantity}} \times 100 \tag{2.7}$$

It is necessary to state clearly to which reagent the excess refers.

Example 2.4

To ensure complete combustion, 20% excess air is supplied to a furnace burning natural gas. The gas composition (by volume) is methane 95% and ethane 5%.

Calculate the moles of air required per mole of fuel.

Solution

Basis: 100 mol gas, as the analysis is volume percentage.

$$\text{Reactions: } CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_2H_6 + 3.5O_2 \rightarrow 2CO_2 + 3H_2O$$

Stoichiometric moles of O_2 required $= 95 \times 2 + 5 \times 3.5 = \underline{207.5}$

With 20% excess, moles of O_2 required $= 207.5 \times 1.2 = 249$

Moles of air (21% O_2) $= 249 \times 100/21 = 1185.7$

Air per mole of fuel $= 1185.7 / 100 = \underline{11.86 \text{ mol}}$

Sources of conversion, selectivity, and yield data

If there is minimal by-product formation, then the reactor costs (volume, catalyst, heating, etc.) can be traded off against the costs of separating and recycling unconverted reagents to determine the optimal reactor conversion. More frequently, the selectivity of the most expensive feeds for the desired product is less than 100%, and by-product costs must also be taken into account. The reactor optimization then requires a relationship between reactor conversion and selectivity, not just for the main product but for all the by-products that are formed in sufficient quantity to have an impact on process costs.

In simple cases, when the number of by-products is small, it may be possible to develop a mechanistic model of the reaction kinetics that predicts the rate of formation of the main product and by-products. If such a model is fitted to experimental data over a suitably wide range of process conditions, then it can be used for process optimization. The development of reaction kinetics models is discussed in Section 15.3 and is described in most reaction engineering textbooks. See, for example, Levenspiel (1998), Froment et al. (2010), Fogler (2016), and Rawlings and Eckerdt (2013).

In cases where the reaction quickly proceeds to equilibrium, the yields are easily estimated as the equilibrium yields. Under these circumstances, the only possibilities for process optimization are to change the temperature, pressure, or feed composition so as to obtain a different equilibrium mixture. The calculation of reaction equilibrium is easily carried out using commercial process simulation programs, as described in Section 4.5.1.

When the number of components or reactions is too large, or the mechanism is too complex to deduce with statistical certainty, then response surface models can be used instead. Methods for the statistical design of experiments can be applied, reducing the amount of experimental data that must be collected to form a statistically meaningful correlation of selectivity and yield to the main process parameters. See Montgomery (2019) for a good introduction to the statistical design of experiments.

In the early stages of design, the design engineer will often have neither a response surface nor a detailed mechanistic model of the reaction kinetics. Few companies are prepared to dedicate a laboratory or pilot plant and the necessary staff to collecting reaction kinetics data until management has been satisfied that the process under investigation is economically attractive. A design is thus needed before the necessary selectivity and yield data set has been collected. Under such circumstances, the design engineer must select the optimal reactor conditions from whatever data are available. This initial estimate of reactor yield may come from a few data points collected by a chemist or taken from a patent or research paper. The use of data from patents is discussed in Section 2.4.1.

For the purposes of completing a design, only a single estimate of reactor yield is needed. Additional yield data taken over a broader range of process conditions give the designer greater ability to properly optimize the design. In process synthesis projects, one purpose of the design may be to set yield targets for a research team, as described in Section 2.6.1.

2.3.4 Recycles and purges

Processes in which a flow stream is returned (recycled) to an earlier stage in the processing sequence are common. If the conversion of a valuable reagent in a reaction process is appreciably less than 100%, the unreacted material is usually separated and recycled.

Separation processes can also be a source of recycles. The return of reflux to the top of a distillation column is an example of a recycle process in which there is no reaction.

The presence of recycle streams makes the calculation of process material and energy balances more difficult. Without recycle, the material balances on a series of processing steps that can be carried out sequentially, taking each unit in turn, with the calculated flows out of one unit becoming the feeds to the next. If a recycle stream is present, then at the point where the recycle is returned, the flow will not be known, as it will depend on downstream flows not yet calculated. Without knowing the recycle flow, the sequence of calculations cannot be continued to the point where the recycle flow can be determined.

Two approaches to the solution of recycle problems are possible:

1. **The cut and try ("tear") method.** The recycle stream flows can be estimated and the calculations continued to the point where the recycle is calculated. The estimated flows are then compared with those calculated, and a better estimate is made. The procedure is continued until the difference between the estimated and the calculated flows is within an acceptable tolerance.
2. **The formal algebraic method.** The presence of recycle implies that some of the mass balance equations must be solved simultaneously. The equations are set up with the recycle flows as unknowns and solved using standard methods for the solution of simultaneous equations.

With simple problems that have only one or two recycle loops, the calculation can often be simplified by the careful selection of the basis of calculation and the system boundaries. This is illustrated in Example 2.5.

The solution of more complex material balance problems involving several recycle loops is discussed in Chapter 4.

Example 2.5

The block diagram in Fig. 2.12 shows the main steps in the balanced process for the production of vinyl chloride from ethylene. Each block represents a reactor and several other processing units. The main reactions are:

***Block* A, chlorination**

$$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2, \text{ yield on ethylenne 98 percent}$$

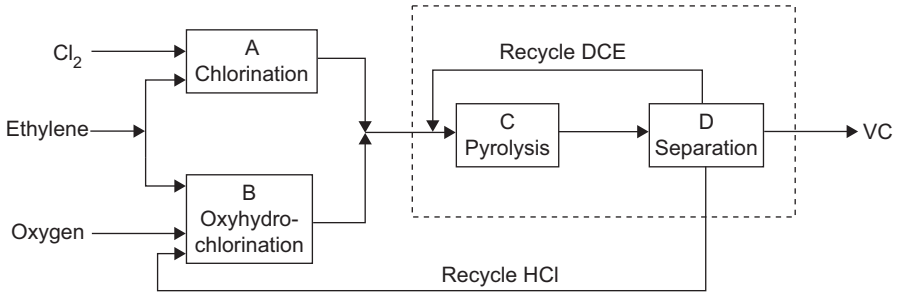


FIG. 2.12 Block flow diagram of balanced process for vinyl chloride (*VC*).

Block B, oxyhydrochlorination

$$C_2H_4 + 2HCl + 0.5O_2 \rightarrow C_2H_4Cl_2 + H_2O, \text{ yields: on ethylene 95\%, on HCl 90\%}$$

Block C, pyrolysis

$$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl, \text{ selectivity of DCE to VC 99\%, selectivity to HCl 99.5\%}$$

The HCl from the pyrolysis step is recycled to the oxyhydrochlorination step. The flow of ethylene to the chlorination and oxyhydrochlorination reactors is adjusted so that the production of HCl is in balance with the requirement. The conversion in the pyrolysis reactor is limited to 55%, and the unreacted DCE is separated and recycled.

Using the yields given, and neglecting any other losses, calculate the flow of ethylene to each reactor and the flow of DCE to the pyrolysis reactor, for a production rate of 12,500 kg/h VC.

Solution

Molecular weights: vinyl chloride 62.5, DCE 99.0, HCl 36.5.

$$\text{VC per hour} = \frac{12{,}500}{62.5} = 200 \text{ kmol/h}$$

Draw a system boundary around each block, enclosing the separation section (block D) and the DCE recycle within the boundary of step C, as shown in Fig. 2.12.

Let the flow of ethylene to block A be X and to block B be Y and the HCl recycle be Z.

Then the total moles of DCE produced $= 0.98X + 0.95Y$, allowing for the yields, and the moles of HCl produced in block C

$$= (0.98X + 0.95Y)0.995 = Z \tag{a}$$

Consider the flows to and from block B. The yield of DCE based on HCl is 90%, so the moles of DCE produced:

$$= 0.5 \times 0.90Z$$

Note: The stoichiometric factor is 0.5 (2 mol HCl per mol DCE).

The yield of DCE based on ethylene is 95%, so

$$0.5 \times 0.9Z = 0.95\,Y$$

$$Z = 0.95 \times 2Y/0.9$$

Substituting for Z into equation (a) gives

$$Y = (0.98X + 0.95Y)0.995 \times \frac{0.9}{2 \times 0.95} \tag{b}$$

$$Y = 0.837X$$

Turning to block C, total VC produced $= 0.99 \times$ total DCE, so

$$0.99(0.98X + 0.95Y) = 200\text{kmol/h}$$

Substituting for Y from equation (b) gives $X = \underline{\underline{113.8 \text{ kmol/h}}}$

and $Y = 0.837 \times 113.8 = \underline{\underline{95.3 \text{ kmol/h}}}$

HCl recycle from equation (a)

$$Z = (0.98 \times 113.8 + 0.95 \times 95.3)0.995 = \underline{\underline{201.1\text{kmol/h}}}$$

Note: Overall yield on ethylene $= \dfrac{200}{(113.8 + 95.3)} \times 100 = \underline{\underline{96 \text{ percent}}}$

The total flow of DCE from blocks A and B is $\frac{200}{0.99} = 202$ kmol/h, but this does not include the recycle. Because the conversion is 55%, if the recycle flow is R, then $202 / (202 + R) = 0.55$; hence the total flow of DCE to the pyrolysis reactor is $202 + R = 202 / 0.55 = 367.3$ kmol/h

Purge

It is usually necessary to bleed off a portion of a recycle stream to prevent the buildup of unwanted material. For example, if a reactor feed contains inert components or by-products that are not separated from the recycle stream in the separation units, these inerts would accumulate in the recycle stream until the stream eventually consisted entirely of inerts. Some portion of the stream must be purged to keep the inert level within acceptable limits. A continuous purge would normally be used. Under steady-state conditions:

$$\text{Loss of inert in the purge} = \text{Rate of feed of inerts into the system}$$

The concentration of any component in the purge stream is the same as that in the recycle stream at the point where the purge is taken off. So the required purge rate can be determined from the following relationship:

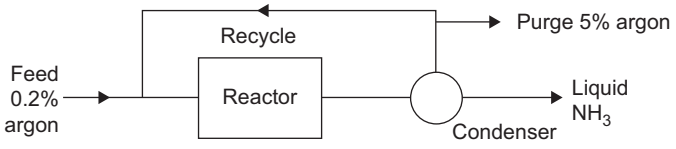
$$[\text{Feed stream flow} - \text{rate}] \times [\text{Feed stream inert concentration}]$$
$$= [\text{Purge stream flow} - \text{rate}] \times [\text{Specified(desired) recycle inert concentration}]$$

Example 2.6

In the production of ammonia from hydrogen and nitrogen, the conversion, based on either raw material, is limited to 15%. The ammonia produced is condensed from the reactor (converter) product stream, and the unreacted material is recycled. If the feed contains 0.2% argon (from the nitrogen separation process), calculate the purge rate required to hold the argon in the recycle stream below 5.0%. Percentages are by volume.

Solution

Basis: 100 moles feed (purge rate will be expressed as moles per 100 mol feed, as the production rate is not given).
Process diagram:



Volume percentages are taken as equivalent to mol%.

Argon entering system with feed $= 100 \times 0.2/100 = 0.2$ mol.

Let purge rate per 100 mol feed be F.

Argon leaving system in purge $= F \times 5/100 = 0.05\ F$.

At the steady state, argon leaving = argon entering

$$0.05F = 0.2$$

$$F = \frac{0.2}{0.05} = \underline{\underline{4}}$$

Purge required: 4 mol per 100 mol feed.

Bypass

A flow stream may be divided and some part diverted (bypassed) around some units. This procedure is often used to control stream composition or temperature.

Material balance calculations on processes with bypass streams are similar to those involving recycle, except that the stream is fed forward instead of backward. This usually makes the calculations easier than with recycle.

2.4 Selection, modification, and improvement of commercially proven processes

Engineers in industry do not usually design a new process from scratch if a commercially proven alternative is available. Companies usually seek to avoid the extra costs and risks inherent in technology commercialization. New molecules are usually made using adaptations of processes that have been shown to work for similar compounds. Even when a brand-new process is contemplated, the design team will usually also prepare a conventional design for comparison.

The use of a proven basic flow scheme does not eliminate innovation from the design. Several alternative designs may already be in commercial practice, each optimized around different feeds, catalysts, or reactor concepts. The design team must evaluate the different designs and optimize each to the local design basis to select the best. The commercial processes may need modification to make the desired product or by-products or to process an unusual feed material. It may be possible to improve the existing technology by substituting one or more unit operations, by using better catalysts or enzymes, by deploying improved separation or reactor technology, or by using different solvents to reduce environmental impact. The scale of production may also cause changes to the flowsheet; for example, if a large new plant requires reactors or separation columns to be constructed in parallel trains.

This section discusses factors a design team should consider when developing a flowsheet based on a commercially proven technology. The special case of developing a flowsheet for the revamp of an existing plant is treated in Section 2.5.

2.4.1 Sources of information on manufacturing processes

This section gives a brief overview of sources of information on commercial processes that can be found in the open literature.

The chemical process industries are competitive, and the information that is published on commercial processes is restricted. The articles on particular processes published in the technical literature and in textbooks invariably give only a superficial account of the chemistry and unit operations used. They lack the detailed information on reaction kinetics, process conditions, equipment parameters, and physical properties that is needed for process design. The information that can be found in the general literature is, however, useful in the early stages of a project, when searching for possible process routes. It is often sufficient for a flowsheet of the process to be drawn up and a rough estimate of the capital and production costs made.

The most comprehensive collection of information on manufacturing processes is probably the *Encyclopedia of Chemical Technology* edited by Kirk and Othmer (2001), which covers the whole range of chemical and associated products. An abridged version of the Kirk–Othmer encyclopedia is also available in paperback (Kirk, 2007). The latest version of the Kirk–Othmer encyclopedia is available through the Wiley online library at http://onlinelibrary.wiley.com. Another encyclopedia covering manufacturing processes is that edited by McKetta (2001). Several books have also been published that give brief summaries of the production processes used for the commercial chemicals and chemical products. The best known of these is probably Shreve's book on the chemical process industries, now updated by Austin and Basta (1998). Comyns (2019) lists named chemical manufacturing processes, with references.

The extensive German reference work on industrial processes, *Ullman's Encyclopedia of Industrial Technology,* is now available in an English translation, Ley, C., (Ed.) (2002).

Specialized texts have been published on some of the more important bulk industrial chemicals, such as that by Miller (1969) on ethylene and its derivatives; these are too numerous to list but should be available in the larger reference libraries and can be found by reference to the library catalogue. Meyers (2016) gives a good introduction to the processes used in oil refining. Kohl and Nielsen (1997) provide an excellent overview of the processes used for gas treating and sulfur recovery.

Many of the references cited here are available in electronic format from Knovel. Most companies and universities have Knovel subscriptions. Access to Knovel is also available to members of professional societies such as the American Institute of Chemical Engineers (AIChE).

Books quickly become outdated, and many of the processes described are obsolete, or at best obsolescent. More up-to-date descriptions of the processes in current use can be found in the technical journals. The journal *Hydrocarbon Processing* publishes an annual review of petrochemical processes, which was entitled *Petrochemical Developments* and is now called *Petrochemicals Notebook*; this gives flow diagrams and brief process descriptions of new process developments.

Patents

Patents can be a useful source of information, but some care is needed in extracting information from them. To obtain a patent, an inventor is legally obliged to disclose the best mode of practice of the invention; failure to do so could render the patent invalid if it were contested. Most patents therefore include one or more examples illustrating how the invention is practiced and differentiating it from the prior art. The examples given in a patent often give an indication of the process conditions used, though they are frequently examples of laboratory preparations rather than of the full-scale manufacturing process. Many process patents also include examples based on computer simulations, in which case the data should be viewed with suspicion. When using data from patents, it is important to carefully read the section that describes the experimental procedure to be sure that the experiments were run under appropriate conditions.

A patent gives its owner the right to sue anyone who practices the technology described in the patent claims without a license from the patent owner. Patent attorneys generally try to write patents to claim broad ranges of process conditions so as to maximize the range of validity and make it hard for competitors to avoid the patent by making a slight change in temperature, pressure, or other process parameters. Very often, a patent will say something along the lines of "the reaction is carried out at a temperature in the range 50° to 500 °C, more preferably in the range 100° to 300 °C and most preferably in the range 200° to 250 °C." It is usually possible to use engineering judgment to determine the optimal conditions from such ranges. The best conditions will usually be at or near the upper or lower end of the narrowest defined range. The examples in the patent will often indicate the best operating point.

Patents can be downloaded for free from the website of the U.S. Patent Office, www.uspto.gov. The U.S. PTO website also has limited search capability. The entire U.S. PTO collection is also available at www.google.com/patents. Most large companies subscribe to more sophisticated patent search services such as Derwent Innovation (www.derwentinnovation.com), PatBase (www.patbase.com), or GetthePatent (www.getthepatent.com).

Several guides have been written to help engineers understand the use of patents for the protection of inventions and as sources of information; such as those by Auger (1992) and Gordon et al. (2017).

Consultants

Engineers in industry often hire specialist consulting firms to prepare analyses of commercial technology. Consultants can be used to provide an impartial assessment of a competitor's or vendor's process. Some consulting firms such as SRI and Nexant regularly publish assessments of the technology available for making different chemicals. These assessments are based on flowsheets and design models that the consultants have developed from information that they gathered from the literature and from direct contact with the technology suppliers.

Some caution is needed when working with consultants. The client must carry out due diligence to ensure that the consultant is truly impartial and does not bias their analysis. The client should also cross-check the information provided by the consultant against recent patents and publications to ensure that the consultant is working from the latest information.

Vendors

Technology suppliers and contractors will sometimes make design information available to a client in the hope of securing a sale. If a project team requires information to make a technology selection, the technology vendors may be willing to supply edited PFDs (for example, with stream flows blanked out or with some information missing), reactor yields, or even designs from a similar plant at a smaller production scale. More detailed information is usually provided by vendors when bidding on a contract for a project that has a high likelihood of going forward.

2.4.2 Factors considered in process selection

Once the design team has assembled information on the alternative commercial processes, they will usually need to carry out substantial customization and optimization of the designs before a selection can be made.

The information given in the open literature is usually restricted to block flow diagrams and (occasionally) reactor yields. The first step is usually to complete a full PFD and mass and energy balance of the process. These can be used for preliminary sizing and costing of the main process equipment to obtain an estimate of the required capital investment, as described in Chapter 7. The feed and product flow rates and energy consumption can be used to estimate the costs of production, as described in Chapter 8. The economic analysis methods introduced in Chapter 9

can then be applied to determine the overall project economics and choose which design gives the best overall economic performance according to the criteria established by the company.

If one process flowsheet has a particular cost advantage, this will usually become clear in the economic analysis. Factors such as feedstock or fixed-cost advantages that can be very important in selecting *between projects* are usually less important when selecting *between flowsheets* within a given project. The selection between flowsheets is usually influenced more by process yields, energy consumption, and capital requirements, and hence is sensitive to catalyst, organism or enzyme performance, and process design and optimization.

In an industrial context, technology vendors or engineering, procurement, and construction (EPC) contractors will often supply detailed PFDs and material and energy balances to a client when invited to bid on a project. Some diligence is always needed in checking the information in proposals and verifying performance claims against the actual performance of recent plants built by the vendor.

Although an economic analysis is always carried out, it is usually not the sole criterion for technology selection. Some other important factors are described next.

Freedom to practice

Freedom to practice is a legal concept that arises from patent law. If a process, catalyst, enzyme, genetically modified organism, or chemical route is patented, it can only legally be used under license from the patent holder. If another company were to use the technology without a license, they would be infringing on the patent, and the patent holder could sue to stop the use and demand damages.

Determination of freedom to practice usually requires the expert advice of patent attorneys. In rapidly evolving new fields it can be difficult to assess, as patent applications typically are not published until 1 to 2 years after they are filed, so a decision may be made to proceed with building a plant before the intellectual property space can be completely mapped. Another complication is that competing technology vendors may have overlapping patents or patents that appear to block features of each other's designs.

All patents are only valid for a fixed term; in the United States at the time of writing this is 20 years from the date the patent was filed. When a patent has expired, anyone is free to practice the technology. Care must still be taken to check that the original technology developer has not made more recent improvements that are still under patent protection. Many conventional processes are no longer protected by patents and can be bought from EPC companies without paying a royalty or license fee.

When a customer licenses technology from a vendor, the vendor will usually indemnify the customer against patent infringement. This means the technology vendor asserts that they have ownership of the technology and freedom to practice and that they will help the customer fight any patent infringement suits brought by their competitors. Technology vendors sometimes minimize the potential for such lawsuits by forming cross-licensing agreements.

Safety and environmental performance

All commercially practiced technologies should meet or exceed the minimum legally acceptable safety standards, but some older processes may no longer have acceptable environmental performance.

An economic analysis will usually not distinguish whether one process is safer or more environmentally acceptable than another. The methods described in Chapters 10 and 11 can be used to make an assessment of process safety and environmental impact.

When assessing commercial technology, visits to existing sites and reviews of their safety and operational performance can also be helpful.

Government and international restrictions

Governments sometimes place restrictions on companies that can influence technology selection. It is fairly common for nationally owned companies in developing countries to be required to maximize use of indigenous technology, equipment, and parts so as to stimulate the development of local engineering industries and reduce hard currency outflows. This may lead a company to develop its own version of an older technology rather than working with a technology vendor or major international company that can supply the latest technology.

International sanctions can also play an important role in process flowsheet selection. Sanctions can disqualify some companies from offering to supply technology and reduce the set of options available. Sanctions can also restrict the availability of feedstocks. During the 1970s and 1980s, South African companies developed many processes for making chemicals from coal in response to the international sanctions aimed at ending apartheid that restricted their ability to purchase crude oil.

Experience and reliability

One of the critical factors in selecting a commercially proven technology is the extent and diversity of operating experience that has been established. If a process has been widely adopted and proven in many locations by different operating companies, then it is likely to be easy to apply in a new plant. A technology that has only been built once or twice may still experience "teething troubles" and be more difficult to implement.

As more operating experience is gained, the company also gains a better understanding of the reliability of the process. If a particular section of the flowsheet or piece of equipment is known to cause reliability problems, this may create a need to modify the equipment design or even make changes to the flowsheet.

2.4.3 Modification and improvement of established processes

All designs evolve over time. Engineers make modifications to improve process economics, safety, reliability, and environmental impact. Most changes will be minor, such as addition of instrumentation or substitution of equipment; however, significant changes in the flowsheet are sometimes needed.

Modifications that are made to an existing commercial plant are known as *revamp designs* and are addressed in Section 2.5. This section describes techniques for modifying an established process for use in a new plant.

Modifications to improve process economics

Improvements in process economics usually come from reduced capital investment or improved cost of production. Designers seeking improvements in process economics usually start by completing a PFD of the existing design and determining the current estimated capital investment and cost of production (see Chapters 7, 8, and 9). The following tactics can then be applied:

- **Improve reactor selectivity and process yield.** Feedstock costs are usually more than 80% of the cost of production, so improving yields gives the biggest impact on process economics. Improved yields usually require the development of more selective catalysts, enzymes, or organisms, or a more effective reactor design, but sometimes a more efficient separation scheme or better purification of a feed or recycle will also improve yield.
- **Improve process energy efficiency.** Energy costs are usually next largest after feedstock costs for chemicals produced on a large scale. Energy costs can be reduced by improving process energy efficiency. Several different approaches to improving process energy use are described in Chapter 3.
- **Improve process fixed costs.** Fixed costs are usually second to feedstock costs in small-scale processes used for fine chemicals and pharmaceuticals manufacture. Fixed costs are described in Section 8.5. Fixed costs can be reduced by making the process more continuous and less labor-intensive and by increasing the plant attainment of batch processes.
- **Reduce capital investment.** Design engineers look for pieces of equipment that can be combined or eliminated to reduce capital cost. In batch plants, this is often done by carrying out several steps in the same piece of equipment. For example, the feed can be charged to a reactor, heated in the reactor, reacted, cooled down, and the product crystallized before pumping out the product as a slurry and repeating the process.
- **Reduce working capital.** Working capital is described in Section 9.2.3. Working capital can be reduced by decreasing inventories of raw materials, work in progress, and consumables. Making a process more continuous and using fewer different solvents in a process both lead to a reduction in working capital.

It can be seen that some of these suggestions contradict each other; for example, "make batch plants more continuous" but "carry out more operations in the same piece of equipment." Lists of design guidelines (known as *heuristic rules*) often contain apparent contradictions. The designer must either choose which rule is most appropriate to the case under consideration using experience and judgment or else carry out a full design and costing of both alternatives. Heuristic rules are discussed further in the context of process synthesis in Section 2.6.4.

Modifications to improve plant safety

Plants can be made more inherently safe by reducing inventories of hazardous materials by making vessels and other plant equipment smaller; substituting less hazardous materials for feeds, solvents, and intermediates; eliminating explosive mixtures and exothermic reactions; eliminating use of operations that are open to the atmosphere; minimizing worker exposure to chemicals; and other methods discussed in Chapter 10.

Improvements in the safety of a design can be quantified using the methods for risk assessment described in Section 10.8.

Modifications to improve plant reliability

When a plant has been in operation for a few years the operators will have a good idea of which plant sections or pieces of equipment lead to the most operational problems, require the most maintenance, and cause the most unplanned shutdowns.

Reliability problems are usually caused by equipment failures. The most common problems are usually experienced with solids-handling equipment, rotating equipment such as pumps and compressors, heat exchangers that are prone to fouling, and instruments and valves. Sometimes, specification of a more reliable piece of equipment can solve a process reliability problem. More often, a flowsheet change is needed, such as designing with two or more pieces of equipment in parallel so that the plant can continue to operate while one is taken offline for repair or cleaning. This approach is commonly applied for pumps, which are relatively cheap and prone to stalling in operation.

Corrosion, erosion, and plugging caused by corrosion products can be major contributors to poor reliability. Methods to address corrosion in design are described in Chapter 6.

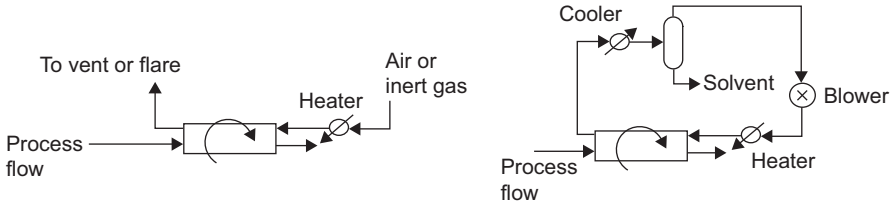
Modifications to improve environmental impact

Many conventional processes were first designed over 40 years ago, when different environmental laws and standards applied. Existing plants may have been modified by addition of end-of-pipe systems for reducing environmental impact; however, changes in the process flowsheet can sometimes achieve the same or better environmental performance at lower cost.

Modifications that are typically used to improve environmental impact include:

- Use of new catalysts, enzymes, or organisms that have better selectivity for the desired product and consequently lead to less waste formation.
- Optimization of reactor design to give better mixing or heat transfer and hence improve reactor selectivity and reduce by-product formation.
- Elimination of solvents or other consumables that become degraded to waste products by the process.
- Elimination of materials that have high environmental impact, such as halogenated solvents, mercury, endocrine disruptors, and compounds that persist in the environment.
- Adoption of closed-loop recirculating gas systems instead of once-through gas flow, thus reducing volatile organic compound (VOC) emissions. For example, Fig. 2.13(*a*) shows a once-through dryer in which the drying gas is vented or sent to a flare, potentially leading to VOC emissions. Fig. 2.13(*b*) shows an alternative design in which a blower is used to circulate the gas. The hot gas leaving the dryer is cooled to allow solvent to be condensed and recovered. There is much less potential for VOC emissions in the closed-loop design, and the consumption of solvent is also reduced.
- Substitution of chemicals with materials that have reduced environmental impact. For example, the cheapest way to neutralize waste sulfuric acid is to react it with lime (CaO) to form gypsum ($CaSO_4$), which is inert and can be sent to a landfill. Instead, if ammonia is used to neutralize the acid, the product will be ammonium sulfate, which can be used as a fertilizer.

Methods for analyzing and reducing the environmental impact of a process are described in Chapter 11.



(a) Rotary dryer with once-through gas flow

(b) Rotary dryer with gas recirculation and solvent recovery

FIG. 2.13 Dryer gas circulation designs.

2.5 Revamps of existing plants

Flowsheet development for plant revamps is a specialized subject in its own right. Revamp design is rarely taught in universities, as revamp studies require access to an operating plant and the data it produces.

Revamps generally fall into two categories. *Debottlenecking* projects are carried out to increase the production rate of a plant while making the same product. *Retrofit* projects are carried out to change the design of a plant to handle different feeds; make different products; exploit better reactor, catalyst, or separation technology; or improve plant safety or environmental impact in response to new regulatory requirements.

2.5.1 Flowsheet development in revamp projects

Fig. 2.14 gives an overall work process for developing a revamp design flowsheet. One of the critical requirements of a revamp project is always to minimize project cost by maximizing reuse of existing equipment. The revamped flowsheet therefore always requires compromises between desired objectives and what can be obtained with the equipment available.

Many features of a revamped flowsheet will be different from the flowsheet of a corresponding new plant. For example, in a revamp it may make sense to add a second distillation column in parallel to an existing column rather than tearing down the existing column and building a new larger one. The use of two small columns in parallel would not be contemplated in a new design. The development of a revamped flowsheet thus requires a lot of information on the performance of existing equipment so that the equipment can be rerated or modified for a role in the new flowsheet. When the existing equipment cannot be upgraded, the designer must find the cheapest method to add new capacity or augment the existing capacity.

Once the revamped flowsheet has been completed, the designers can assess the costs of the new components that must be added. The cost of revamping a plant should always be compared with the cost of building a new plant from scratch. The revamp will usually be a cheaper method for adding small increments of capacity, but for larger capacity increases, a new unit will become more attractive.

The steps in developing a revamped process flowsheet are described in the following sections. Although there is a great deal of retrofit and revamp activity in the chemical industry, particularly in regions such as the United States

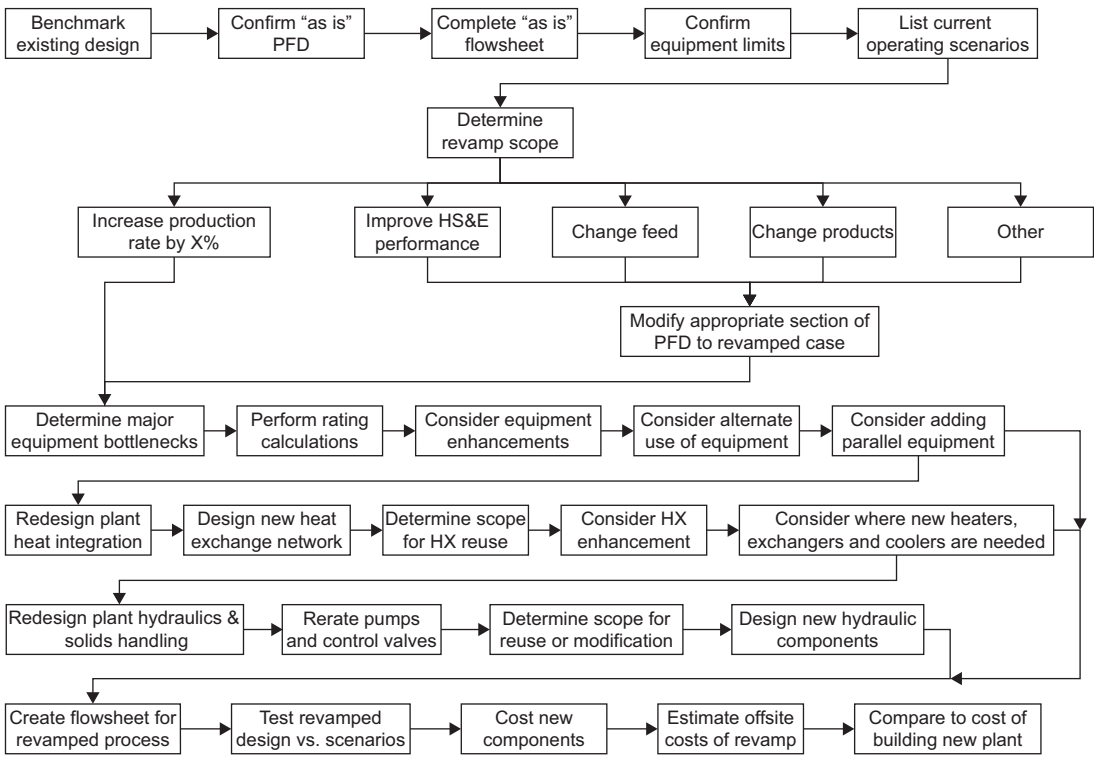


FIG. 2.14 Steps in revamp design.

and European Union, where the industry has been long-established, the authors are not aware of any comprehensive reference works on the subject. The books by Briggs et al. (1997) and Douglas (1988) contain short sections on revamp design. Process revamps for energy savings are discussed in detail by Zhu (2014).

2.5.2 Major equipment debottlenecking

In a revamp design, the capacity of existing equipment determines whether additional equipment must be added in series or parallel, and hence plays a major role in determining the revamped design flowsheet.

Most major equipment is initially specified with a design factor or margin of 10% to 20%; see Section 1.6. This overdesign allows for errors in the design data and methods, but also creates some room for potential expansion of capacity. When a plant is considered for revamp, some of the equipment may still be operating below its full capacity.

The general procedure for equipment debottlenecking follows the steps shown in Fig. 2.14. Once a mass and energy balance has been established for the existing plant, a simulation model of the equipment can be built. The model can then be tested under the proposed new process conditions to determine if the equipment is fit for the new service. For equipment that is difficult to model (for example, centrifuges, fired heaters, and dryers) a specialist or the original equipment vendor may need to be consulted. After establishing the maximum capacity that the equipment can attain while maintaining specifications, modifications to improve capacity can be considered. If it is not possible to satisfy the desired process duty with modifications to the existing equipment, then the cheapest means of adding capacity must be established. This may include complete replacement of the original equipment, with reuse of the original equipment elsewhere in the process.

Some specific examples of techniques for equipment debottlenecking are given next. Revamp of heat transfer equipment is discussed in Section 2.5.3, and revamp of hydraulic and solids handling equipment is described in Section 2.5.4.

Reactor debottlenecking

Reactors are designed with a specified residence time that has been determined to give a desired conversion. For reactors that use a fixed bed of catalyst, this is usually expressed instead as a space velocity:

$$\tau = \frac{V}{v} \tag{2.8}$$

$$SV = \frac{v}{V_{cat}} \tag{2.9}$$

where: τ = residence time
SV = space velocity
V = reactor volume
V_{cat} = fixed bed catalyst volume
v = volumetric flow rate

Space velocity is usually given on an hourly basis and defined on the basis of gas phase flow (GHSV = gas hourly space velocity), liquid phase flow (LHSV = liquid hourly space velocity), or total mass flow (WHSV = weight hourly space velocity = kg/h feed per kg of catalyst inventory). Any consistent set of units can be used for residence time and space velocity.

Equations 2.8 and 2.9 clearly show that an increase in flow rate must lead to a proportional change in either volume, residence time, or space velocity. Adding volume usually requires building additional reactors, so unless the reactors are very inexpensive, the revamp design will focus on ways to reduce residence time or increase space velocity while trying to maintain the same conversion, if possible, so as to minimize the impact on the separation and recycle sections of the plant.

An increase in space velocity or decrease in residence time can be obtained by increasing temperature; backing off on conversion; reducing the concentration of diluents; or using a more active catalyst, enzyme, or organism. Increasing temperature and reducing diluents or solvents (if any are present) will generally lead to worse selectivity and increased cost elsewhere in the process. Many fixed-bed catalytic processes are operated on a temperature cycle, where the reactor temperature is slowly increased over a 1- to 10-year period to compensate for catalyst deactivation and the catalyst is then replaced at the end of the cycle. In such cases, raising the temperature shortens the catalyst run length and requires more frequent plant shutdown. Reducing the reactor conversion also creates additional cost

elsewhere in the process as the amount of unreacted feed recycle is increased. Improving the catalyst performance is often the least expensive way to boost capacity, and the availability of new catalysts often sets the scope for revamp projects.

An additional problem with revamping fixed-bed catalytic reactors is the effect of reactor pressure drop. The pressure drop across a packed bed is proportional to the flow rate squared, so pressure drop increases rapidly as flow rate is increased. Approaches that can be taken to reduce reactor pressure drop include rearranging series reactors into parallel flow (Fig. 2.15) and converting down-flow reactors to radial flow (Fig. 2.16). (A more detailed drawing of a radial flow reactor is given in Chapter 15; see Fig. 15.29). With packed beds that are in up-flow, care must be taken to avoid fluidizing the catalyst in the revamped design. If the up-flow velocity is close to the minimum fluidization velocity, then the reactor should be converted to down-flow or replaced with a larger reactor. Sizing of packed bed reactors is discussed in more detail in Section 15.7.3.

When it is necessary to add reactor capacity, a technique that is widely used is to add a pre-reactor to the existing reactor sequence, as in Fig. 2.17. Because a pre-reactor typically runs at low conversion, it can be operated under conditions that would not normally be good for selectivity; for example, at higher temperature or with less solvent or diluent. This makes the pre-reactor more volume-efficient than the existing reactor sequence, without compromising on overall selectivity.

When a detailed model of the reaction kinetics, including side reactions, is available, more complex reactor networks can be designed that give improved selectivity and yield of desired products. A revamp project can then add reactor capacity to bring the reactor section performance closer to that of the ideal reactor network. The design of reactors and reactor networks is discussed in more detail in Chapter 15.

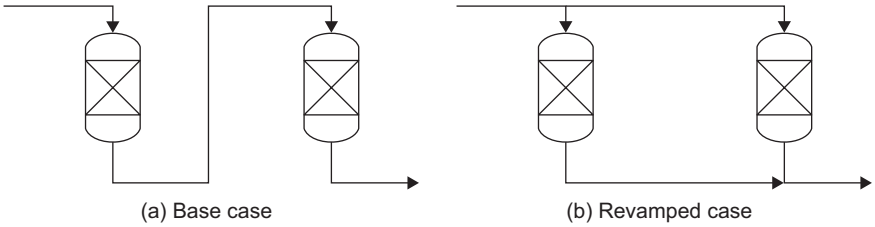


FIG. 2.15 Series to parallel reactor revamp.

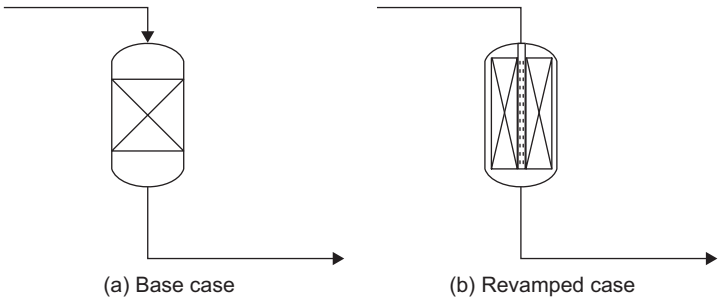


FIG. 2.16 Down-flow to radial-flow reactor revamp.

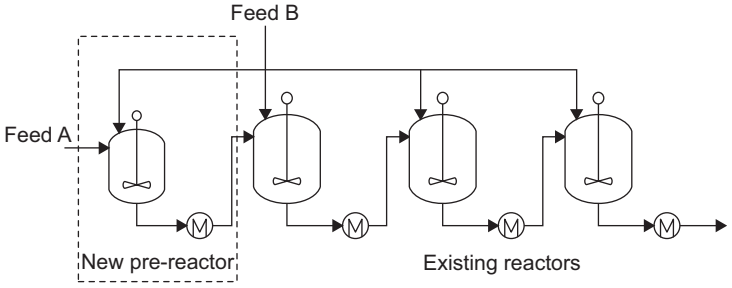


FIG. 2.17 Reactor revamp using a pre-reactor.

Separation column debottlenecking

The capacity of separation columns is usually limited by column hydraulics; see Section 17.13. If the feed flow rate increases, the vapor rate in the column increases proportionately, and at some point the column will flood and become inoperable. Two approaches can be taken to obtain more capacity:

1. Increase the open area for vapor flow to delay the onset of flooding.
2. Increase the number of stages in the column by using high-efficiency trays or trays that allow a closer tray spacing, so that the reflux ratio, and hence vapor rate, can be reduced.

Both of these methods are used by separation tray and packing vendors, and there are many proprietary designs of high-efficiency, high-capacity trays and packing on the market. When revamping a column, the common practice is to contact the tray and packing vendors, who will then supply an estimate of how many trays must be replaced to achieve a desired capacity. It is often not necessary to re-tray the entire column. The detailed design of distillation columns is discussed in Chapter 17.

When it is necessary to add capacity to a distillation column and the use of high-capacity trays is not sufficient, a prefractionator scheme is sometimes used, as illustrated in Fig. 2.18. The prefractionator makes a preliminary separation of the feed that reduces the reflux requirements of the main column. A revamped prefractionator is usually provided with its own reboiler and condenser to avoid increasing the load on the main column reboiler and condenser.

Another common tactic in debottlenecking separation sections is to reuse the existing distillation columns in a different application. If a plant has three or more columns, then a revamp can be carried out by building one new column to replace the largest of the existing columns, revamping the largest old column to replace the second largest, etc. In this context, largest refers to the largest diameter, which governs vapor rate and capacity. If the columns do not have sufficient height for the new application, they can be re-trayed with high-efficiency internals or combined in series. In some cases, particularly for relatively short low-pressure columns, it may even make sense to add height to a column by welding on a new top section.

2.5.3 Revamp of heat exchange networks

The heat exchangers, heaters, and coolers of a plant will cause many of the bottlenecks to plant expansion. When a plant is revamped to a new purpose, such as changed feed or products, the existing heat recovery system will no longer be optimal and may no longer make good sense. The common practice in major revamps is to complete the revamp design of the other major equipment first, then address the heaters, coolers, and exchangers subsequently, as shown in Fig. 2.14.

The design of heat recovery systems and heat-exchanger networks is covered in Chapter 3. Chapter 19 addresses the detailed design of heat exchangers, heaters, and coolers. Revamp of a complex heat-exchange system should

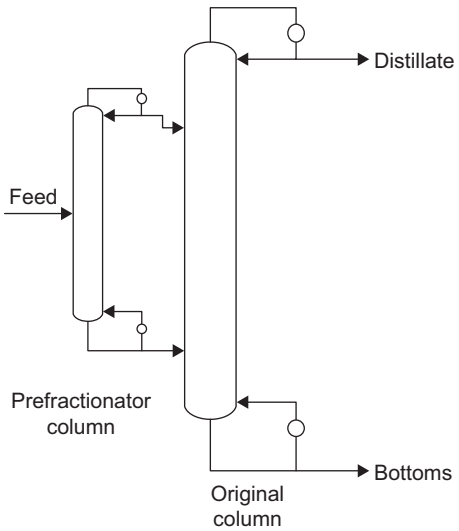


FIG. 2.18 Distillation column revamp using a prefractionator.

always be treated as a network problem rather than by revamping each item individually, as the lowest-cost solution will always be that obtained by optimizing the system as a whole.

The revamp of heat-exchanger networks has been the subject of much research, and very effective techniques and software for heat-exchange network revamp have been developed. The *network pinch* method developed by Asante and Zhu (1997) is now the most widely used method in the industry. This method has been automated (Zhu and Asante, 1999) and is used by most of the companies that offer heat integration consulting services. Smith (2016) gives a concise overview of the network pinch approach; see also Zhu (2014).

For simple processes with only a few heaters and coolers, the tactics described in the following sections can be used.

Heat exchangers

For a heat exchanger:

$$Q = UA\Delta T_m \tag{2.10}$$

and

$$Q = m_i C_{p,i} \Delta T_i \tag{2.11}$$

where : Q = heat transferred per unit time, W
U = the overall heat-transfer coefficient, W/m^2K
A = heat-transfer area, m^2
ΔT_m = the mean temperature difference, the temperature driving force, °C
m_i = the mass flow rate of stream i, kg/s
$C_{p,i}$ = the specific heat capacity of stream i, J/kgK
ΔT_i = the change in temperature of stream i for a stream that undergoes only sensible heat changes, °C

Increasing the flow rate increases the required duty and therefore requires an increase in heat transfer coefficient, area, or effective temperature difference.

The correlations that are used to predict heat transfer coefficients for sensible heat transfer are usually proportional to $Re^{0.8}$, where Re is the Reynolds number, which is proportional to flow rate. Hence, the process-side transfer coefficient increases almost in ratio to the increase in flow unless the exchanger is boiling or condensing the process stream. For heaters and coolers, it may therefore be possible to reuse the exchanger in the same service if an increase in utility-side heat transfer coefficient or a change in utility temperature can make up the rest of the required duty. This is topic explored in Example 2.7.

One of the first and most important steps in revamping a heat exchange system is to benchmark the current system and estimate the heat transfer coefficients that are currently being obtained. If these are substantially lower than expected from the original design of the process, this may indicate fouling, plugging, or other problems that should be addressed during the revamp.

There are several proprietary methods for enhancing the performance of tubular exchangers. Tube inserts such as hiTRAN, TURBOTAL, and Spirelf can be used to increase turbulence and tube-side heat transfer coefficient. Low-fin tubes can be used to increase shell-side effective area (Wolverine, 1984; see also Section 19.14). Reboiling and condensing coefficients can be increased by use of UOP High Flux or High Cond tubing.

Plate exchangers usually do not require enhancement methods. Gasketed plate exchangers are very easy to revamp, as more plates can simply be added to the exchanger; see Section 19.12. Welded plate exchangers are not amenable to the use of inserts or to expansion by adding plates.

Heaters and coolers

The techniques described for heat exchangers apply equally well to steam or oil heaters and water coolers. Decreasing cooling water return temperature (by increasing cooling water flow rate) and raising hot oil temperature are widely used methods in plant revamps.

Fired heaters are usually difficult to revamp and require the involvement of heater and burner specialists. If there is space in the heater, additional tubes can be added. Similarly, if there is space in the convective section, it can be used for pre-heat to off-load some of the furnace duty. In some cases, the addition of improved burners will allow more uniform heating and higher average tube-wall heat flux. Fired heater design is discussed in more detail in Section 19.17.

Air coolers (Section 19.16) are also difficult to revamp. The designer does not have the ability to specify a lower ambient temperature! Common air cooler revamps include:

- Adding more banks of tubes and installing more powerful fans.
- Adding water-spray systems to increase cooling capacity on the hottest days.
- Water-spray systems are effective, but can increase air-side fouling over time.

Example 2.7

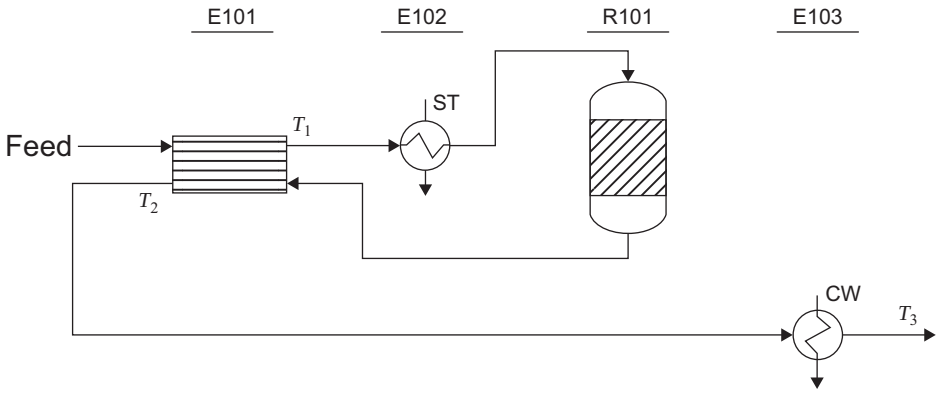
Fig. 2.19 shows a simple heat-exchange system. A feed stream is heated by heat exchange in a plate exchanger and then further heated in a steam heater before entering a fixed-bed reactor. The product from the reactor is cooled in the plate exchanger and then further cooled using cooling water. Exchanger specifications and current performance are given in the figure. Propose modifications to the system to allow a revamp to 50% higher capacity.

Solution

Start with the plate heat exchanger, E101. A 50% increase in flow through the exchanger would give a $(1.5)^2 = 2.25$ factor increase in exchanger pressure drop. If this was acceptable, then assuming that the heat transfer coefficient is proportional to $Re^{0.8}$:

$$\text{New heat transfer coefficient} = 350 \times (1.5)^{0.8} = 484 \text{ W/m}^2\text{K}$$

Assuming the reactor operates at the same outlet temperature, we can make heat balances for the base case and revamp case.



Exchanger	E101	E102	E103
Type	Plate	S&T	S&T
Duty (kW)	800	400	200
Hot side T in (°C)	140	180	60
Hot side T out (°C)	60	180	40
Cold side T in (°C)	40	120	25
Cold side T out (°C)	120	160	35
F_t factor	1	1	0.92
Hot side heat transfer coefficient (W/m^{2}K)	700	2000	700
Cold side heat transfer coefficient (W/m^{2}K)	700	500	700
Overall heat transfer coefficient (W/m^{2}K)	350	400	350
Area (m^2)	114	27.5	31.7
ΔT_{lm}	20	36.4	19.6

FIG. 2.19 Heat-exchange system for Example 2.7.

Base case:

$$Q_{101} = 800 \times 10^3 = m_f C_{p,f}(120-40) = m_p C_{p,p}(140-60)$$
$$m_f C_{p,f} = m_p C_{p,p} = 10^4$$

Where subscript f denotes feed and p denotes product.

Revamp case:

$$Q_{101} = 1.5 m_f C_{p,f}(T_1-40) = 1.5\, m_p C_{p,p}(140-T_2)$$
$$T_1 = 180 - T_2$$

and

$$Q_{101} = UA\Delta T_m = 484 \times 114 \times (140-T_1)$$

So

$$1.5 \times 10^4 (T_1-40) = 484 \times 114 \times (140-T_1)$$

hence

$$T_1 = 118.6^\circ\text{C}$$
$$T_2 = 61.4^\circ\text{C}$$

So we only lose 1.4 degrees of heat exchange as long as the increase in pressure drop that results from the higher flow rate is acceptable.

Now look at the steam heater, E102. In the revamp case:

$$Q_{102} = 1.5 \times 10^4 (160-118.6) = 621 \text{ kW}$$

The heat transfer coefficient is only increased on the process (cold) side:

$$\text{New cold} - \text{side coefficient} = 500 \times (1.5)^{0.8} = 691.6 \text{ W/m}^2\text{K}$$
$$\text{New overall heat transfer coefficient} = \left((2000)^{-1} + (691.6)^{-1}\right)^{-1} = 513 \text{ W/m}^2\text{K}$$

(Overall heat transfer coefficient calculated using Equation 19.2)

So for the exchanger to be feasible, we would need to raise the steam temperature to T_s, where:

$$Q_{102} = UA\Delta T_m$$
$$621 \times 10^3 = 513 \times 27.5 \times \left(\frac{(T_s-160)-(T_s-118.6)}{\ln\left(\frac{T_s-160}{T_s-118.6}\right)}\right)$$
$$T_s = 186.5^\circ\text{C}$$

So the heater remains viable if the steam temperature can be increased by 6.5 °C. This might be accomplished by raising the local pressure of the medium pressure steam system, for example, by making adjustments in the steam pressure regulator valve set points. If that was not possible, and if the heater was rated for a sufficiently high pressure, then high-pressure steam could be considered instead of medium-pressure steam.

Turning to the cooler, E103. In the revamp case:

$$Q_{103} = 1.5 \times 10^4 (61.4-40) = 321 \text{ kW}$$

To meet this extra duty we need to increase the cooling water flow rate by a factor F_{cw}, which changes the cooling water outlet temperature to T_w, where:

$$Q_{103} = 321 \times 10^3 = F_{cw} \times 20 \times 10^3 (T_w-25)$$

and

$$321 \times 10^3 = UAF\Delta T_{lm}$$

For the revamp case, the logarithmic mean temperature difference ΔT_{lm} depends on T_w and the overall heat transfer coefficient will be:

$$\frac{1}{U} = \frac{1}{700 \times (1.5)^{0.8}} + \frac{1}{700 \times (F_{cw})^{0.8}}$$

These equations must be solved iteratively. This is easily done using a spreadsheet, giving:

$$F_{cw} = 1.89$$
$$T_w = 33.5^\circ\text{C}$$

The exchanger would be feasible if we could accept this increase in cooling water flow rate; however, such a large increase would give a very large increase in pressure drop. The pressure drop is proportional to flow rate squared and so would increase by a factor $(1.89)^2 = 3.57$, which would probably not be acceptable.

An alternative approach for E103 is to see what the outlet temperature would be if cooling water flow were limited. Suppose the cooling water flow cannot be increased more than 20%, giving a 44% increase in pressure drop. If we allow the cold outlet temperature and hot outlet temperature to vary, the same spreadsheet model can be solved to give:

$$T_w = 36.4^\circ\text{C}$$
$$T_3 = 43.1^\circ\text{C}$$

So in this case the designer would have to consider whether the product stream could be made 3.1 °C hotter, which depends on the downstream processing.

If this option was also unacceptable, the designer would have to consider adding another cooler. A simple approach would be to split the hot stream, leaving E101 into two streams in a ratio of 2:1. The larger stream could still be sent to E103, and the smaller one could be sent to a parallel cooler half the size of E103. This option would not push the operation of E103 much beyond the current operating mode.

In summary, one option that would allow a 50% increase in throughput would be:

- **E101:** No change, as long as the factor 2.25 increase in pressure drop is acceptable on hydraulic review.
- **E102:** Increase steam temperature to 186.5 °C; no capital modification is needed.
- **E103:** Consider accepting a 3.1 °C warmer product. If this is unacceptable, add a new exchanger E104, half the size of E103, in parallel to E103 and split the hot stream, leaving E101 in a 2:1 ratio between E103 and E104.

Alternatively, if E101 is a gasketed plate heat exchanger (see Section 19.12.1), the designer could also consider adding more plates to increase the area available in E101. We can increase the plates in E101 until we achieve the same channel velocity and pressure drop as the base case then solve the remaining problem for E102 and E103, or, alternatively, increase the plates in E101 until the existing E102 and E103 are able to satisfy all of the remaining heating and cooling load without modifications. This alternative solution is explored in Problem 2.11. The addition of plates to E101 would be more expensive than just altering a few temperatures, but would most likely be less costly than adding E104 and could even be cheaper than making the hydraulic modifications necessary to cope with a large increase in pressure drop.

2.5.4 Revamp of plant hydraulics

Any revamp project that leads to increases in plant throughput will have a significant effect on the plant hydraulic equipment. Because pressure drop is proportional to velocity (and hence flow rate) squared, a 40% increase in flow is sufficient to double the pressure drop. The introduction of parallel equipment in the flowsheet may also create a need for additional control valves to regulate flow in the desired ratios, which adds more pressure drop to the plant. Adding equipment to modify the process also has an impact on the hydraulic design.

Much of the design effort in revamp projects goes into evaluating and redesigning the plant hydraulics. All of the pump-and-line calculations and control valve sizing calculations must be repeated for the revamped design case. It is usually not cost-effective to replace the piping with new pipe of more optimal diameter, so usually the designers will accept a higher pressure drop in the pipes and process equipment and then redesign the pumps and control valves accordingly.

The design of pumps, compressors, piping systems, and control valves is discussed in more detail in Chapter 20. The following sections provide some specific guidelines relevant to revamp flowsheet development.

Compressors

Compressors are the largest and most expensive items in the plant hydraulic equipment. Compressor design is covered in more detail in Section 20.6. Because compressors are expensive to replace, experienced designers usually try to reuse the existing compressors in the new flowsheet.

The relationship between flow rate and pressure delivered depends on the type of compressor (Fig. 2.20), but the pressure delivered will usually decrease if the compressor operates at higher flow. The only exception to this rule is large reciprocating compressors, which are usually designed with a recycle from the product to the feed, known as a *spill-back*. If the spill-back flow is large enough, some increase in flow can be obtained by reducing the spill-back, with no loss in delivered pressure.

When two compressors are used in parallel, the total flow increases, but the delivered pressure cannot be greater than the lower pressure delivered by either compressor; see Fig. 2.21. When two compressors are used in series, the pressure delivered increases, but the flow rate does not; see Fig. 2.22.

In a revamp flowsheet design, the designer seeks to increase the pressure delivered to overcome the increased plant pressure drop, as well as an increase in flow rate. From Figs. 2.21 and 2.22 it can be seen that the only way to increase both the pressure delivered *and* the flow rate while adding only one compressor is somewhat paradoxically to *reduce* the flow rate in the existing compressor so that it delivers a higher pressure and then add a second machine in parallel, as shown in Fig. 2.23. The extent to which the flow rate can be reduced depends on the type of compressor and current operating conditions. In this scenario, the revamped flowsheet would need to show two

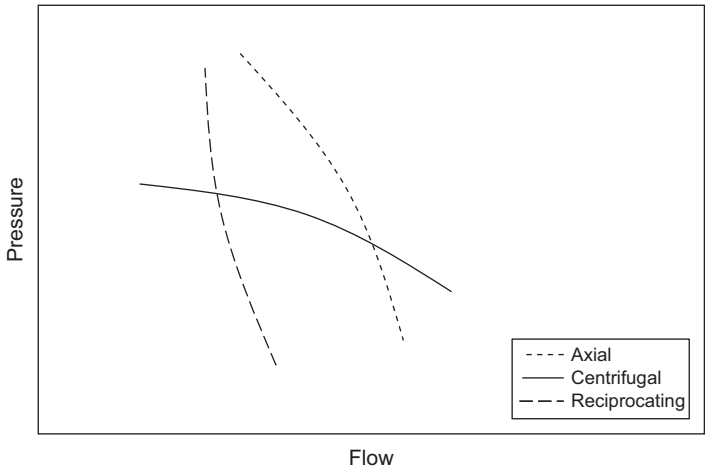


FIG. 2.20 Pressure–flow rate curves for different compressor types.

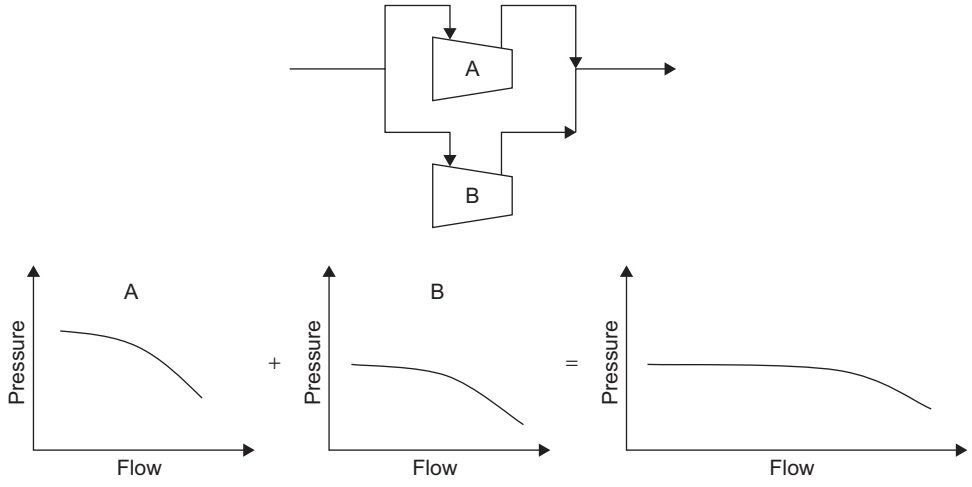


FIG. 2.21 Compressors in parallel.

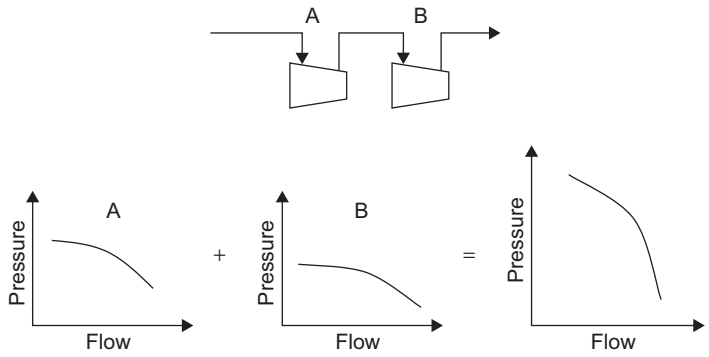


FIG. 2.22 Compressors in series.

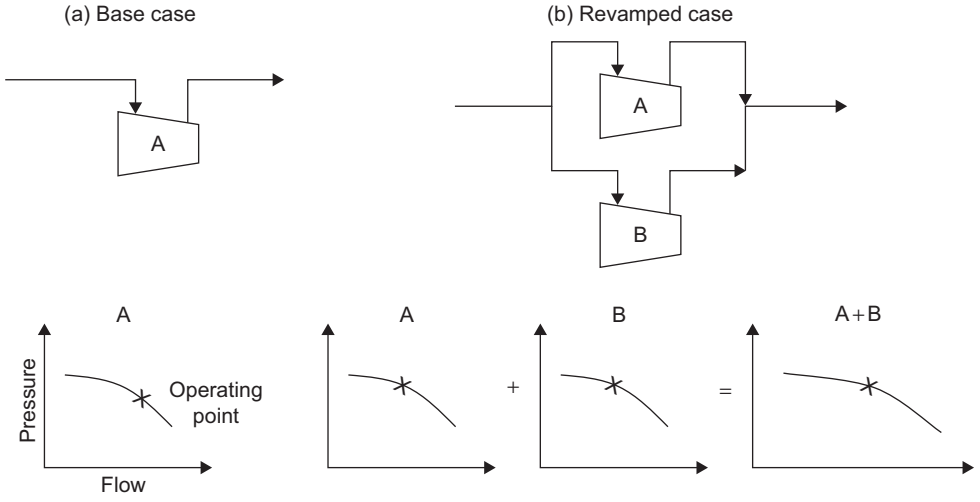


FIG. 2.23 Compressor revamp.

compressors in parallel. A revamp from one machine operating at 100% flow rate to two similar machines in parallel, each at 70% flow rate, would give an overall 40% increase in flow.

If it is not possible to meet the desired flow and pressure with the addition of only one new compressor, it will usually be preferable to replace the existing compressor rather than adding new compressors in series and parallel.

If a compressor cannot be reused in its current location in the revamped flowsheet, it should be evaluated for other process uses. Air compressors and blowers should also always be reevaluated and can be used to assist heaters, boilers, dryers, or even site instrument air systems if there are no suitable process uses.

Pumps

Pumps are relatively inexpensive compared with compressors and will often be replaced entirely in a revamp. Pumps are discussed in more detail in Section 20.7.

The most commonly used pumps are centrifugal pumps. Centrifugal pumps exhibit pressure-flow behavior similar to that shown for centrifugal compressors in Fig. 2.20. A typical pump curve is given in Fig. 20.15. The same pump can deliver a set of different performance curves depending on the impeller diameter and motor speed. The designer can therefore sometimes obtain the required performance just by selecting new impellers for the existing pumps.

Control valves

All control valves must always be rated to confirm that they are correctly sized for the revamped design case and will give the desired controllability, turndown, and ability to meet different operating scenarios. Control valve design and sizing are discussed in Section 20.11.

When parallel equipment is introduced into the revamped flowsheet, the design engineers must determine how the flow is to be split between the existing and new equipment. A simple T-junction or branch will often not be effective, as the rate of fouling or pressure-drop accumulation of the new and old equipment will not be the same, even if they have the same capacity and design, and flow would then preferentially go through one piece of equipment, leading to poor performance of both. The desired split ratio is rarely 1:1 and may need to be adjusted once the plant is put into operation. The most common approach is to put a new control valve on the branch that leads to the new equipment. The existing equipment is likely to be limited by pressure drop, so the new equipment can be designed with lower pressure drop to allow for the pressure drop associated with the control valve. A less costly, but less effective, alternative is to use a manual valve or even a restriction orifice in the bypass line and make manual adjustments until the desired flow ratio is obtained.

Control valves that act discontinuously and handle low flow rates will sometimes be suitable for reuse in the revamped plant as long as the new actuation rate is acceptable. Control valves on main plant flows will usually need to be replaced, as will control valves on gas or vapor streams. The revamped flowsheet does not need to indicate which existing valves are reused and which are replaced, but should show all new control valves that are added.

2.6 Synthesis of novel flowsheets

The terms *process synthesis* and *conceptual process design* are used for the invention of completely new process flowsheets. As stated previously, very few entirely new designs are developed commercially because of the high financial risks inherent in using unproven technology. The primary goals of process synthesis are therefore to reduce commercialization risk and to maximize economic attractiveness so as to generate sufficient financial reward to balance the risk.

Process synthesis has been the subject of a great deal of academic and industrial research over the past 40 years. Many problems that were previously solved using inspired guesswork can now be formally posed and optimized. The use of process simulation programs has also made it much easier to evaluate and optimize alternative flowsheets; see Chapter 4 for more on process simulation. Several prominent researchers in the field of process synthesis have written textbooks on process design that strongly emphasize process synthesis. These are listed in the bibliography at the end of this chapter. Several excellent books have been written on process synthesis in its own right: Rudd et al. (1973); Douglas (1988), and El-Halwagi (2006), as well as on aspects of process synthesis, such as distillation sequencing (Doherty and Malone, 2001), mass integration (El-Halwagi, 2017), and heat integration (Kemp, 2007; Shenoy, 1995). Although it is beyond the scope of this book to cover all aspects of process synthesis, this section sets out an overall framework for flowsheet synthesis that addresses the key issues encountered in developing and commercializing new processes. The reader is encouraged to read the books listed here and in the bibliography for more insights into the subject.

2.6.1 Overall procedure for flowsheet synthesis

Most efforts to systematize process synthesis begin by setting out a sequence or hierarchy of steps for the designer to follow. Design hierarchies recognize that some steps need to come before others and should guide the designer to eliminate unattractive options and focus effort on designs that are most likely to be successful.

The most intuitively obvious design hierarchy is the so-called *onion diagram*. Fig. 2.24 shows a version of the onion diagram given by Smith (2016). The onion diagram represents a design starting with the reactors; adding separation and recycle systems; then proceeding to add heat recovery, utility systems, and environmental systems. Rudd et al. (1973) proposed a more theoretically abstract synthesis hierarchy that essentially follows the same steps but included an additional step of integrating reaction, mixing, separation, or change of state tasks into unit processes or operations.

Douglas (1988) set out a somewhat different approach, summarized in Table 2.1. Douglas emphasized early introduction of process economics to guide the elimination of weaker alternatives, with continuous refinement of the economic model as more detail is added to the flowsheet. This is a useful approach, as it can highlight deficiencies in the design at an early stage.

The reality of process development in industry is usually a lot less systematic than the idealized picture painted by academic researchers. In industrial practice, process development is more interdisciplinary, more iterative, and much less linear than the simple synthesis models suggest. The flowsheet synthesis step is usually part of a larger

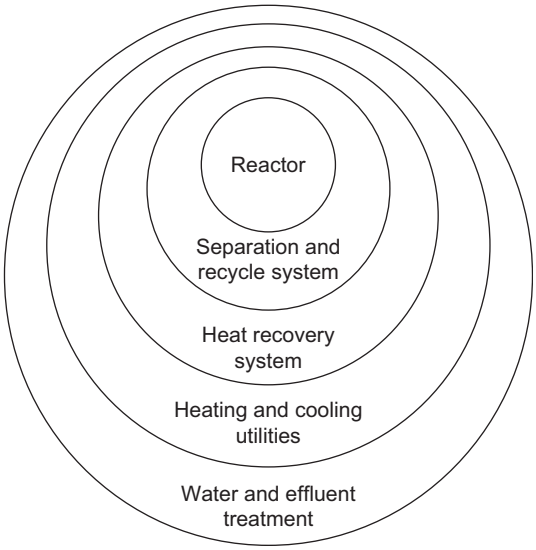


FIG. 2.24 Onion diagram. *From Smith, R. [2016].* Chemical process design and integration *[2nd ed.] Wiley.*

TABLE 2.1 Hierarchy of process synthesis decisions

1. Batch vs. continuous
2. Input–output structure of the flowsheet
3. Recycle structure of the flowsheet
4. General structure of the separation system
   a. Vapor recovery system
   b. Liquid recovery system
5. Heat exchanger network

Data from Douglas, J. M. (1988). Conceptual design of chemical processes. *McGraw-Hill.*

effort that involves chemists, biologists, and other engineers and includes laboratory and pilot plant experiments to determine reactor performance and establish yields and product recoveries. The engineers working on synthesis seldom have all the data that are needed to properly optimize the design and often must guide the research members of the team to collect additional data under conditions that will be more favorable to process economics. Many industrial processes involve multiple reaction steps carried out in sequence with intermediate separation steps, and it may be difficult to assess the performance of later steps without good information on the nature and quantity of by-products that are carried over from earlier steps in the sequence. The design team therefore needs to form a rough impression of the PFD and economics, using minimal information on process chemistry, so as to develop an understanding that can guide the efforts of the research team.

Fig. 2.25 sets out an approach to flowsheet synthesis that sets flowsheet development in the context of working with a research team to establish yields and reactor performance. The Douglas hierarchy and onion diagram form substeps in this procedure, as described next.

Step 1. Initial economics

The very first step should be to collect prices for feeds and products and confirm that the cost of production will be attractive if a stoichiometric yield is obtained. If the cost of feed is more than the product value, then there is no hope of developing an economically attractive process and the work should be stopped unless the team has strong evidence that prices will change in the future. This step is particularly important when assessing nontraditional feeds; for example, when looking at processes for converting food-based renewable feeds into chemicals.

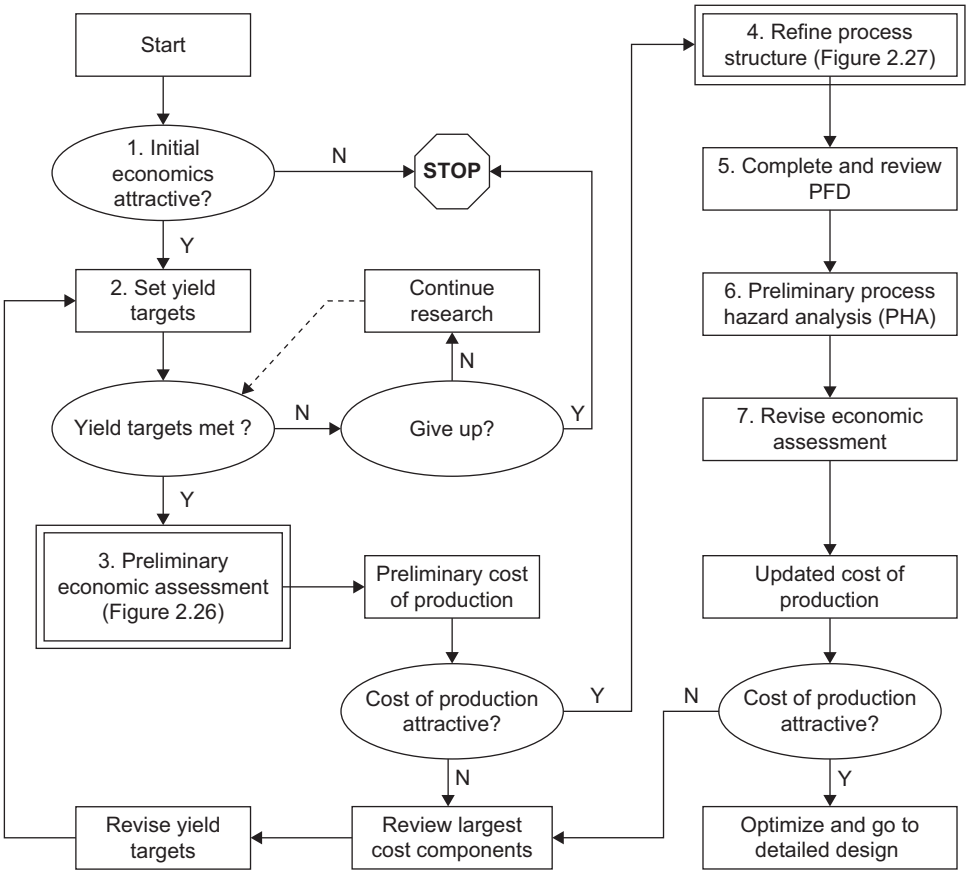


FIG. 2.25 Procedure for process synthesis.

Step 2. Set yield targets

The research team needs to set realistic targets that will lead to an attractive process. The term *yield targets* includes targets for by-product selectivity as well as main product selectivity and conversion. Methods for setting and revising yield targets are given in Section 2.6.3. The researchers will generally need to carry out process development experiments to optimize reactor conditions and catalyst, enzyme, or organism performance to meet the yield targets.

On the first pass through the procedure, the designers may choose to just accept whatever yields and selectivities the research chemists or biologists have already established. When more information on process economics has been generated, the targets can be revised and improved.

If the yield targets are not met, the company must make a strategic decision on whether to continue or abandon the research. Research discoveries are often serendipitous and can be hard to plan. Companies often choose to allow a low level of research activity to continue over a long period once clear success criteria have been established.

Step 3. Preliminary economic assessment

The goal of a preliminary economic assessment is to arrive at a preliminary estimate of the cost of production once the yield targets have been met. The substeps in carrying out a preliminary economic assessment are illustrated in Fig. 2.26. This procedure is similar to that of Douglas (1988), but it should be emphasized that less detail is put into the design and the goal is not to arrive at a PFD or even a detailed block flow diagram at this point.

The components of cost of production and methods for calculating each component are discussed in detail in Chapter 8. For most processes, 80% or more of the cost of production will be feedstock cost minus credits for any economically viable by-products. The rest of the cost of production is chiefly made up of utility costs (mostly energy), fixed costs (mostly labor), and annualized payments to generate an expected return on the capital investment. The split between these depends on the type and scale of the process. Small-scale batch processes will have a higher proportion of fixed costs, whereas large-scale petrochemicals or solids-handling plants will have a higher proportion

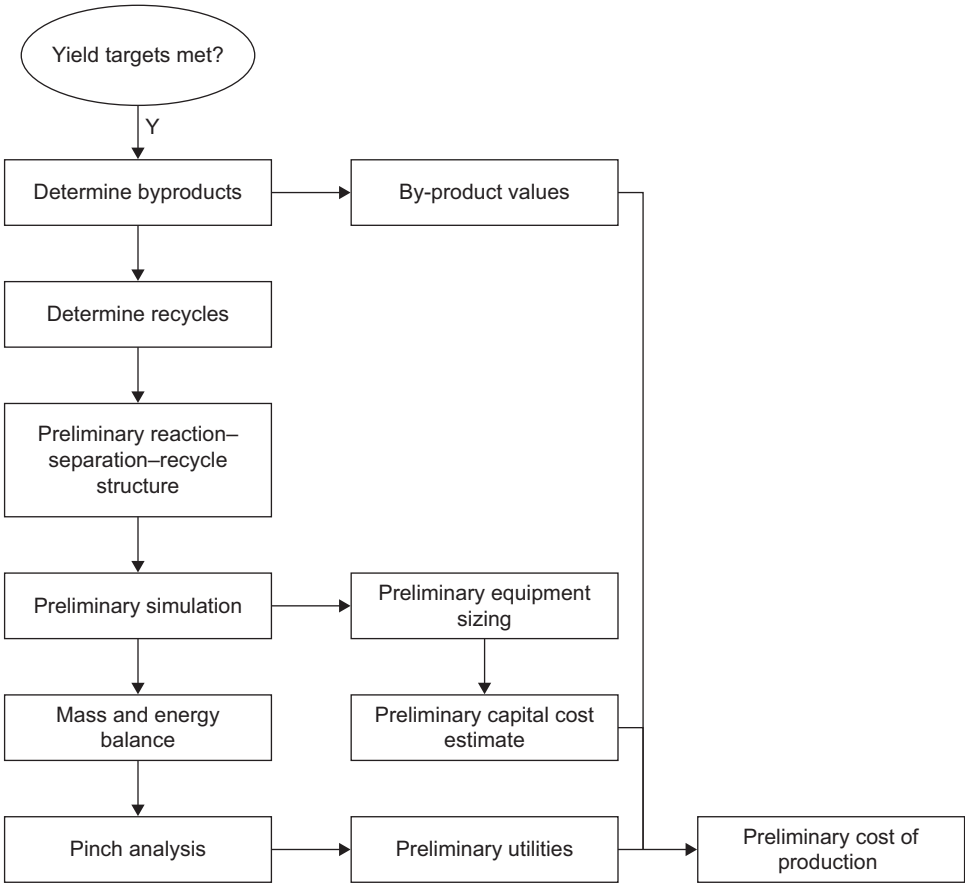


FIG. 2.26 Preliminary economic assessment.

of utility costs. In a preliminary economic assessment, the designer seeks to make a quick estimate of these major components of cost, and hence determine whether the process will be able to make product at an attractive price.

The first step is to look at the yields and identify any significant by-products. By-products can be formed by the reaction stoichiometry, by side reactions, or from extraneous components in the feeds. By-products must be refined and sold, treated as waste streams, or recycled to extinction in the process. A quick examination of the yields and prices of the by-products is usually sufficient to establish which are suitable for recovery. The economic assessment of by-product recovery is discussed in more detail in Section 8.2.3.

Once the designer has a notion of which by-products are worth recovering and which by-products must be recycled, a preliminary reaction−separation−recycle structure can be sketched. It is not important to have the best or optimal flowsheet at this point, and the design team may want to propose a few alternatives to see which is least costly. A process simulation model can then be built and used to generate a mass and energy balance and obtain rough sizing of the major process equipment. The preliminary simulation should include all recycles, reactors, and separation equipment and should capture all changes in temperature and pressure. It does not need to include a heat recovery design and should use heaters and coolers instead of heat exchangers whenever there is a change in temperature. The use of commercial programs for process simulation is discussed in Chapter 4. The preliminary simulation model does not have to be built using a commercial simulation program, but it will usually be convenient to do so, so that the model can be extended as the flowsheet is subsequently refined.

The preliminary equipment sizes from the simulation model (or hand calculations) can be used to develop an initial estimate of the capital cost of building a plant. Estimation of capital costs is covered in Chapter 7. The capital cost is then annualized so that it can be added to the other costs of production. Annualization of capital costs is covered in Section 9.7. In a preliminary economic assessment, the designers usually annualize capital costs by dividing by 3. The basis for this rule of thumb is set out in Section 9.7.2.

The process energy consumption and utility costs are difficult to assess without completing a process simulation and energy balance. Most processes have significant opportunity to reduce energy costs by heat recovery, so simply

adding up all the heating and cooling duties would be a gross overestimate. Instead, a first estimate of energy consumption can be made by carrying out the targeting step of pinch analysis to get hot and cold utility targets. Pinch analysis and other heat recovery methods are described in Chapter 3. At this point in the design it is not necessary to design the heat recovery system, as the targets are adequate for the preliminary economic assessment.

The preliminary estimates of main product and by-product production rates, feed and energy consumption, and capital cost can be used to make a preliminary estimate of the cost of production, as described in Chapter 8. If the cost of production appears attractive, the design team proceeds to the next step. If not, the economic assessment can be used to highlight the major components of cost that must be reduced to make the process economically interesting. Having identified the cost components that must be addressed, the design team can either look at alternative flowsheets that reduce these costs or else set more aggressive yield targets and go back to the research stage.

Step 4. Refine process structure

If the preliminary economic assessment indicates that the process is potentially economically attractive, then it is important to develop a complete PFD and make sure that no costs have been overlooked. The steps in completing a more rigorous design are shown in Fig. 2.27. It can be seen that these follow roughly the same sequence as the onion diagram of Fig. 2.24.

The first step is to optimize the reaction–separation–recycle structure of the flowsheet and confirm the yields under the optimal conditions. The preferred conditions can be estimated by optimization of the preliminary simulation model and economic model. Additional experimental data may be needed if the optimal conditions are different from the conditions originally proposed. The reactor designs must be tested and yields confirmed in the presence of recycle streams, which may require construction of a pilot plant that can operate in recycle mode. The design of reactors is described in Chapter 15.

The design of the separation systems encompasses not only those separations associated with product recovery and recycles but also feed purification, product purification, and by-product recovery. The design of separation processes is covered in detail in Chapters 16, 17, and 18. In some cases, product purification or by-product recovery will require additional reaction steps. For example, in the recovery of ethylene produced by steam cracking of light hydrocarbons, it is easier to hydrogenate by-product acetylene than to separate it by distillation (Fig. 2.28).

When the by-product separation and recovery sections have been designed in more detail, the attractiveness of recovering the by-products can be revisited. If the costs of producing the by-products are excessive, the designer should revisit the reaction–separation–recycle structure or return to the preliminary economic analysis step.

When designing the reaction and separation steps, as much use as possible should be made of proven process subsections. If a particular reaction, separation, recovery, or purification step is already practiced commercially, then the same method will probably be least costly and will most likely have the least technical risk for the new design. Borrowing proven concepts from established technology is one of the most effective strategies for reducing commercialization risk. Some caution is needed when applying this strategy if the new case is not identical to the commercially proven design, and the designer should take particular care to ensure that slight differences do not lead to potential safety or operability issues. The designer must also ensure that there are no active patents on the features that are borrowed so that there is freedom to practice them.

Once the major process equipment has been specified, the design team should have a good idea of the stream temperature and pressure requirements, and the heat recovery system can be designed. Process heat recovery is described in Chapter 3, and heat transfer equipment is covered in Chapter 19.

The designs of the plant hydraulics and control system are interlinked, as control valves introduce additional pressure drop into the process and can create a requirement for additional pumps. Once the major equipment, including heat exchangers, has been specified, a preliminary PFD can be drafted, which can be developed into a full PFD by adding the location of control valves, pumps, and compressors. The design of plant control systems and location of control valves is discussed in Chapter 5. The design of hydraulic equipment is covered in Chapter 20, and solids handling systems are described in Chapter 18. When all the equipment has been added to the PFD, the process simulation can be updated to produce mass and energy balances to complete the flowsheet. The PFD is then ready for review.

Step 5. PFD review

Review of a PFD is one of the most important steps in flowsheet development. A full PFD review is always carried out in design, regardless of whether the process is a revamp or new unit, or whether it uses novel or proven technology. This vital step is discussed in more detail in Section 2.7.

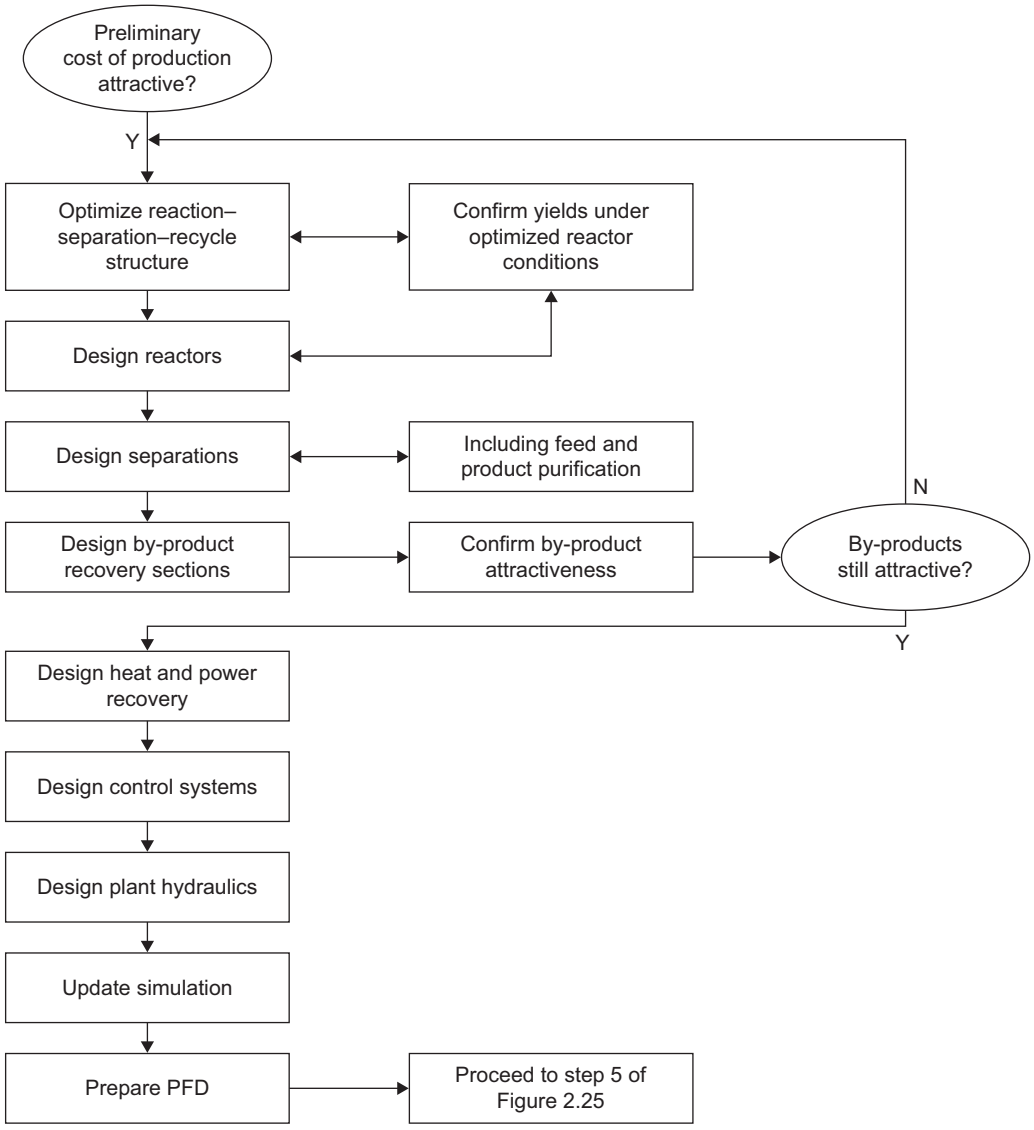


FIG. 2.27 Refining the process flowsheet.

Step 6. Preliminary process hazard analysis

When a completed PFD and mass and energy balance are available, a preliminary process hazard analysis (PHA) can be carried out. A PHA will identify major hazards inherent in the process and may indicate a need to alter some process conditions, substitute different equipment, or completely redesign sections of the process. If the preliminary PHA identifies major modifications to the PFD, the design team should go back to the relevant stage of the procedure and generate a safer alternative design. The role of safety in design is discussed in detail in Chapter 10.

Step 7. Revise economic assessment

The completed PFD and mass and energy balance allow the design team to make more accurate designs of the process equipment, and hence arrive at more accurate estimates of the capital cost and cost of production. If the process still appears to be attractive, then it may be worth developing as an investment, and other methods of economic assessment will be used to determine a viable project for implementing the technology; see Chapter 9. The models that have been developed now have sufficient accuracy to enable more rigorous optimization and can be used as a starting point for detailed design of the plant and equipment. Optimization methods in process design are discussed in Chapter 12.

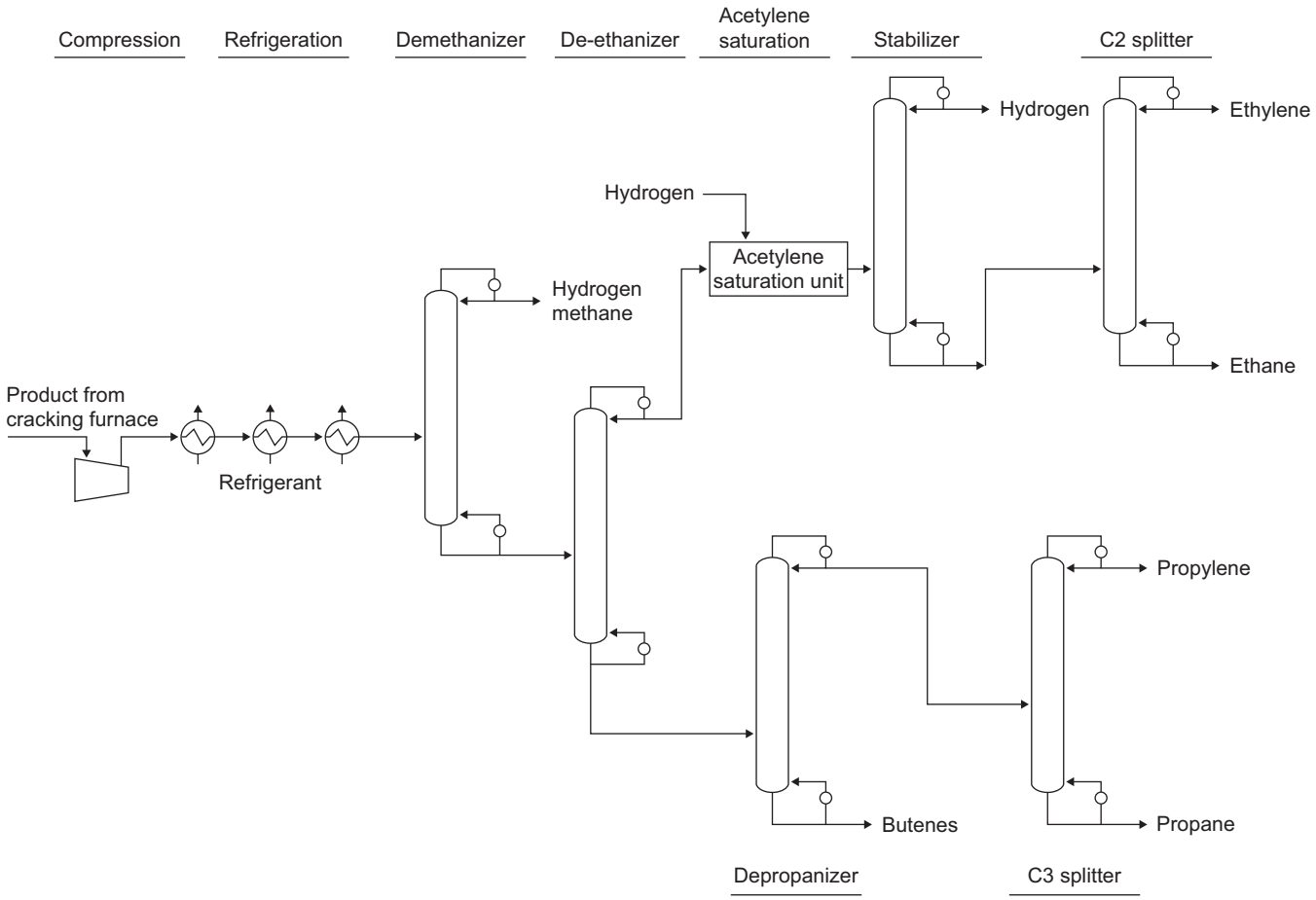


FIG. 2.28 Ethylene recovery from steam cracking.

If the updated cost of production is no longer attractive, the added detail can be used to further define the major cost components and identify areas for process improvement. This will often involve reducing by-product and recycle handling, and hence translate into setting tougher yield targets.

2.6.2 Economic analysis in process synthesis

In process synthesis it is important to use economic analysis to inform decision-making at every step. The procedure outlined in Fig. 2.25 begins with a rough economic analysis and then adds detail to this analysis as information is accumulated. Like an artist beginning with a rough pencil sketch and then filling in details and adding colors, the process design engineer needs to have an overall sense of the composition before getting into the details.

The procedure set out in Fig. 2.25 has three economic check points at steps 1, 3, and 7, corresponding to the initial, preliminary, and updated estimates of the cost of production. At these check points the estimated cost of production should be compared with the product sales price that the marketing organization has forecasted. Usually, the criterion for success will be that the cost of production must be low enough to ensure an acceptable return on the capital deployed. Forecasting of prices and calculation of cost of production are covered in Chapter 8, and methods of economic analysis are described in Chapter 9. Although these three steps in the procedure are formal checks, experienced designers do not wait until the check point to calculate process costs. As soon as information is developed, its impact on the cost of production should be determined. In general, costs accumulate as detail is added to the design, so the design team wants to be aware of large costs as early as possible so that they can start considering alternative design features.

Companies usually use other economic analysis methods, such as net present value (NPV) and internal rate of return (IRR), instead of cost of production when assessing capital investment projects; however, very few companies launch a capital project without having already completed the process synthesis. At the synthesis stage, cost of production is the most useful economic measure, as it is very easily factored into components such as raw material

costs, by-product values, energy costs, etc. Understanding the components of cost of production can help the design team focus on areas of high cost if the target cost of production is not achieved.

2.6.3 Use of targets in process synthesis

Design engineers use targets as a means of setting bounds on design performance that can quickly eliminate unattractive options. Targets also help designers and researchers to focus their efforts on areas that will most effectively improve economic performance. Several different types of targets are used in the synthesis procedure set out in Figs. 2.25, 2.26, and 2.27:

- The cost of production is compared with a price target set by the marketing organization at steps 1, 3, and 7.
- The design team sets targets for the research team at step 2.
- Hot and cold utility targets calculated by pinch analysis are used for initial estimates of process energy consumption.
- The preliminary economic analysis sets targets for capital cost and the components of cost of production that the design team must confirm as they refine the process structure and fill in the PFD.

The basis for targets should always be clearly stated. Whenever possible, targets should be calculated from economic criteria, and the assumptions in the calculations should be made explicit. For example, a badly stated yield target would be:

> "Find me a catalyst that doesn't make by-product X."

A better way of stating this target might be:

> "If reactor selectivity to by-product X is <0.5% of selectivity to the main product, we can eliminate a separation and purification section of the process, with expected 15% savings in capital cost and 20% savings in energy cost."

Targets must not be unrealistically tough, or they will never be achieved and will not be taken seriously. Lenient yield targets are usually not as problematic, as they tend to lead to failure at the preliminary economic assessment stage and are then revised to something more realistic. Lenient targets for cost of production are dangerous, as they allow the design to go forward, and much time and effort can be wasted before harsh economic reality kills the project. Good price forecasting and market analysis are critically important in setting the cost of production targets. These topics are discussed in Chapter 8.

It is important to understand whether a target should be treated as a hard constraint or a soft constraint. Companies sometimes address this question by providing *must-have* targets that are hard constraints and *should-have* targets that are soft constraints. The design team can then reject designs that do not meet the hard constraints, but keep concepts that come close to the soft targets. Soft and hard targets are explored in Example 2.8.

Example 2.8

The marketing group is planning to launch a new product and has forecasted that the mean price for the product will be 5 $/kg, normally distributed with standard deviation 40 ¢/kg. The cost of the stoichiometric amount of feed required to make the product is 3 $/kg. Propose preliminary targets for cost of production and yields.

Solution

If the forecast is accurate and the mean product price is 5 $/kg, then there is a 50% probability the project will have economic success if the cost of production (including capital recovery) is 5 $/kg. Using the standard deviation given in the forecast, we can form the following table:

Cost of production (COP), $/kg	Probability of success
3.80 (= 5 − (3 × 0.4))	99.9%
4.20 (= 5 − (2 × 0.4))	97.7%
4.60 (= 5 − (1 × 0.4))	84%
5.00	50%
5.40 (= 5 + (1 × 0.4))	16%

We can note immediately that this process would pass the initial economic assessment even if we chose a target cost of production with 99.9% chance of success.

The probability of success that we require depends on how risk averse or aggressive the company is. A 98% chance of success might be too conservative and would give a high chance that the project would not meet the targets. A 50% chance of success would probably be too aggressive and would allow the project to go forward and spend money with low likelihood of financial success. As a compromise, management might set a *must-have* target for COP of 4.60 $/kg, with a *should-have* target of 4.40 $/kg. Note that we are not constrained to using integral multiples of the standard deviation in setting the targets; for example, a price target of 4.34 $/kg (= 5 − (1.65 × 0.4)) corresponds to 95% probability of success and would be equally easy to justify as a *must-have* or *should-have* target.

The COP target can now be translated into preliminary yield targets. In Section 2.6.1 it was stated that feed costs are typically at least 80% of COP. Using this rule of thumb, we can state:

$$\text{Target feed cost} = 0.8 \times \text{target COP}$$

The yield targets obviously depend on the number of feeds, the relative costs of individual feeds, and the number of reaction and product recovery steps. From Equations 2.4 and 2.6 we know:

$$\text{Yield} = \frac{\text{product formed}}{\text{stoichiometric product formed}}$$

so:

$$\text{Target plant yield} = \frac{\text{stoichiometric cost /kg}}{\text{target feed cost /kg}}$$

So if the target COP is 4.60 $/kg:

$$\text{Target plant yield} = \frac{3}{0.8 \times 4.60} = 0.815$$

Note that this is the target yield over all the steps in the process. If we assume that we lose roughly 5% of the product during all the steps of product recovery and purification, then:

$$\text{Target plant yield from reactors} = \frac{0.815}{0.95} = 0.858$$

If we have two reaction steps and one feed is more expensive than the others, we could further decompose the yield target into targets for each step:

$$\text{Target plant yield from reactors} = Y_1 Y_2$$

where Y_1 and Y_2 are yields of reaction steps 1 and 2. We could set equal targets for each step:

$$Y_1 = Y_2 = \sqrt{(0.858)} = 0.926$$

or we could use our knowledge of process chemistry or biology to define a suitable allocation between the steps.

Note that the targets calculated are plant yields, not reactor yields. If costly unconverted feeds can be recycled, the plant yields translate into reactor selectivity targets, not reactor yield targets (see Section 2.3.3).

Note also that even in this simplistic example, the apparently very favorable economics quickly translated into rather tough targets for reactor performance.

2.6.4 Use of heuristic rules in process synthesis

Heuristic is an adjective meaning "of, or pertaining to, or based on, experimentation, evaluation or trial and error methods," which pretty much sums up most engineering knowledge. The terms *heuristic rules* and *design heuristics* are commonly used to describe rules of thumb and design guidelines that have been developed based on experience. Experience is good, but it is rarely acquired instantly or bought cheaply. Design guidelines based on generalizations are only useful if the designer has sufficient experience to understand when to apply the guideline and when to make an exception.

There is often confusion about what constitutes a design heuristic. Consider the following statements, most of which have been made in this chapter:

1. *"The heat of condensation of steam is about 2000 kJ/kg."*
2. *"Pressure drop is usually proportional to velocity squared."*
3. *"Feedstock costs are typically at least 80% of the total cost of production."*
4. *"Capital costs can be annualized by dividing by 3."*
5. *"When designing reaction and separation steps, use proven process subsections as much as possible."*

Statement 1 is a convenient data approximation. It is accurate within ±10% for saturated steam over a temperature range from 100 °C to 240 °C, which covers most temperatures at which steam is used for process heating. Remembering this fact may save an engineer some time when carrying out hand calculations, but it does not provide any guidance for design.

Statement 2 is a convenient summary of several correlations for pressure drop. It may be very useful for making quick calculations in revamp designs, but again provides no guidance for design.

Statement 3 is a generalization that can be useful as a rough check on cost of production calculations. As illustrated in Example 2.8, it can also be used as a basis for setting initial targets in process synthesis. It is, however, rather too general to provide guidance in design.

Statement 4 is one way of annualizing capital costs. It would be equally valid to state "*Capital costs can be annualized by dividing by 2*" or "*…by dividing by 5,*" depending on the assumptions made. The basis for deriving these numbers is given in Section 9.7.2.

Statement 5 is clearly a design guideline based on a general desire to minimize the number of unproven concepts in the flowsheet.

Although all of these statements are useful as rules of thumb and can help make quick calculations to assess a design, only statement 5 actually provides guidance on how to design a process. It might be useful for an engineer to recall approximate data and generalizations, and several compilations of such rules of thumb have been written (Fisher, 1991; Hall, 2017; Hicks & Chopey, 2012), but these are only helpful in process design when making quick calculations in meetings.

Some design texts provide extensive lists of rules of thumb and selection guidelines. That approach is not adopted here, as heuristics easily lose their meaning when taken out of context. For example, one design text gives the rule for vessel design: "*optimal length to diameter ratio = 3.*" This is questionable even for horizontal and vertical flash drums (see Section 16.3), but is clearly nonsense when wrongly applied to reactors and distillation columns. Inexperienced engineers often have difficulty determining when to apply such heuristic rules, so in this text all shortcut calculations, convenient approximations, and design guidelines will be presented and explained under the relevant design topic.

The most important heuristic rule, which should always be followed, is:

> "Never use a heuristic rule unless you understand where it came from and how it was derived."

2.6.5 Role of optimization in process synthesis

Optimization methods are used in process synthesis to select the best flowsheet options, process conditions, and equipment sizes. The designer must be reasonably sure that design alternatives have been optimized before selecting between them. Optimization underpins all design decisions, and the subject is addressed in more detail in Chapter 12.

The problem that is often encountered when applying optimization methods in process synthesis is that insufficient data are available to properly formulate an optimization problem. For example, it would be good to optimize reactor performance as soon as possible, but the research team may not yet have collected data in the presence of recycle streams or at conditions close to the optimal reactor conditions. Under the circumstances, the designer must optimize the design with the data available and then revisit the optimization later when more data have been collected and the reaction kinetics model has been updated.

Most processes are too complex to formulate a single optimization problem that includes all possible structural flowsheet variations, as well as all continuous process variables. Instead, different aspects of flowsheet synthesis are usually treated as separate optimization tasks. It is important, however, to have an overall optimization model that

captures the major design trade-offs. The cost of production model developed in the preliminary economic assessment can serve as an initial model for optimization. The optimization of subproblems is discussed in Section 12.5.

2.7 PFD review

The most important step in developing a process flowsheet is for the PFD to be rigorously reviewed. This is true regardless of whether the flowsheet is for an established design, a revamp, or a newly invented process. The purpose of a PFD review is to review the design decisions and assumptions and ensure that the flowsheet is complete and shows *all* the equipment needed to really operate the process.

A PFD review is usually attended by the design team and a few outside experts. These may include:

- Senior managers
- Technical experts on process design
- Technical experts on process chemistry, catalysis, or biology
- Equipment or plant design experts
- Process safety experts
- Metallurgists
- Plant operations staff
- Plant mechanical engineers
- Process control engineers

Some companies have rules and procedures governing who must be present at a PFD review, but the review can be effective with only a few people as long as they engage actively with the team.

2.7.1 PFD review procedure

A PFD review is usually carried out as a group exercise. A large printout of the PFD is typically taped or pinned to a wall so that the group can mark up corrections, notes, and other revisions as the review proceeds. The PFD is usually drawn well spaced out to leave room for additions, and may run to several sheets of drawings. One member of the group takes notes and documents any actions that are agreed to or concerns that are raised. If the heat and material balances and stream conditions are not shown on the PFD, printouts are usually provided for the reviewers.

For complex processes, a PFD review may begin with a brief overview of the process chemistry and block flow diagram to establish the context for the reviewers. In some cases the design basis assumptions are also reviewed at the start.

The main part of a PFD review is a "walk through" of the process by the process design engineer. Starting with one feed stream, the designer follows the stream from storage through all the process operations that it encounters. At each process operation, the designer explains the purpose of the operation, the design criteria, and the resulting condition of the stream at the exit. For example, the feed section shown in Fig. 2.29 would be described as follows:

> Feed of 99% pure technical grade A leaves floating roof storage tank T101 through line 101 at ambient conditions. The governing ambient temperature for heater design is winter low temperature of −5 °C and for pump design is summer high temperature of 30 °C. Stream 101 is pumped by centrifugal pump 101 to a pressure of 10 bar gauge, forming stream 102. Pump 101 has a standby spare, shown. Flow of feed A is regulated by flow control valve FCV100, with design pressure drop 1.3 bar. Stream 103 exits FCV100 and is sent to steam heater E101. The purpose of heater E101 is to heat feed to the reaction temperature of 180 °C. High-pressure steam at 240 °C is used as heat source. The steam rate is controlled by temperature controller TC101, which receives input from temperature indicator on the process stream, leaving E101 in Stream 104. The steam has been placed tube side in E101 because the process stream is nonfouling and steam is at high pressure, so this is expected to lead to the lowest-cost design. A pressure drop allowance of 0.7 bar has been assigned to E101. Stream 104 leaves E101 at the desired reactor feed temperature of 180 °C and at reactor pressure 8 bar gauge and enters reactor R1.

As the designer steps through the PFD, the review group asks questions to challenge the design assumptions and identify potential missing equipment. In the previous example, some relevant questions could have been:

- Is it necessary to pass the feed through a filter before FCV100 to remove any crud that accumulated in the tank or came in with the feed?
- Why use high-pressure steam to heat all the way from ambient temperature? Couldn't process heat recovery be used for at least part of the heating?

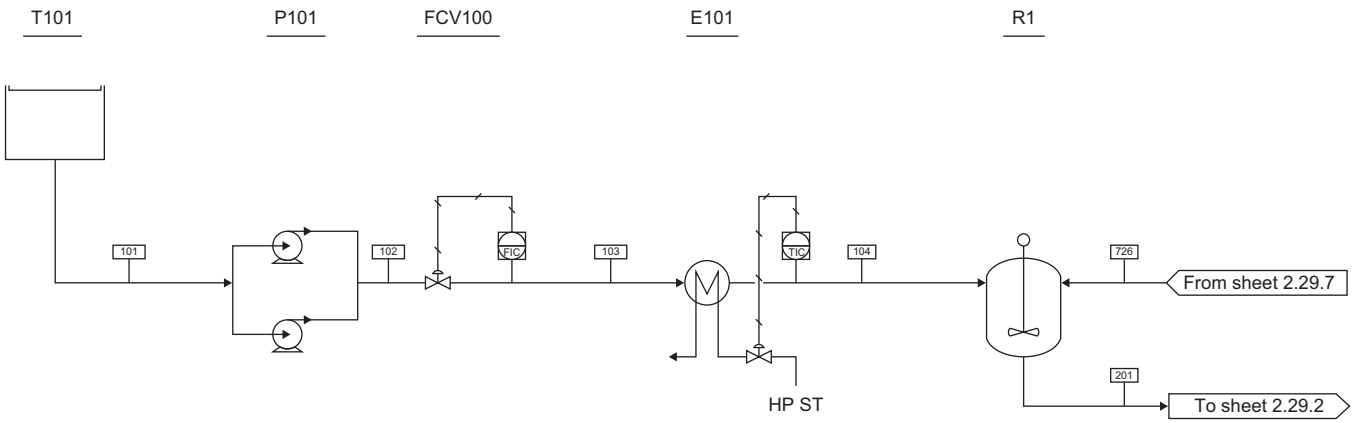


FIG. 2.29 Feed to a reactor.

- Why not use low-pressure steam to heat to 110 °C then high-pressure steam to final temperature?
- Should FCV100 be a separate control loop? Shouldn't it be in ratio to other reactor feeds?
- Did the team look at using a variable-speed drive on the pump to regulate flow instead of a pump and control valve? This would give lower energy consumption.
- What was the basis for choosing 180 °C and 8 bar gauge as the reactor conditions?
- Does the feed need to enter the reactor at reactor conditions? Would a colder or hotter feed reduce the reactor cooling or heating duty?

Some additional typical PFD review questions are given in Table 2.2.

If the questions lead to modifications to the flowsheet that are immediately obvious and agreed to by all the reviewers, then these are marked up as corrections. If further analysis is required before deciding on a modification, it is noted as a follow-up action for the team.

The same procedure is followed for every stream in the PFD. Because it is often necessary to jump from one drawing or section of the flowsheet to another and back again, it is a good idea to mark streams with a highlighter when they have been completed so that the group does not overlook any streams.

Sufficient time must be allowed to complete the PFD review to the satisfaction of all the reviewers. The amount of time needed depends on the complexity and novelty of the design and the familiarity of the reviewers with the technology. For complex designs, a full PFD review can take several days to complete.

2.7.2 PFD review documentation and issue resolution

The notes taken at a PFD review usually include a long list of items that require follow-up by the design team. It is a good idea to include these notes and a description of how any issues and concerns were resolved in the design documentation. The notes should be circulated to meeting attendees immediately after the PFD review meeting to ensure that all issues were correctly captured.

If a PFD review indicated a need for substantial modification of the flowsheet, the group should reconvene after the modifications have been made to review the modified PFD. In process synthesis projects, several rounds of PFD review may be necessary.

2.8 Overall procedure for flowsheet development

Fig. 2.30 shows an overall strategy for flowsheet selection and development. The chart in Fig. 2.30 will generally lead to the selection of a commercially proven process or a modification of such a process when one exists. This reflects the commercial reality that very few business leaders are willing to risk a large sum of money (and their career and reputation) on unproven technology unless the financial return is very good and *no good alternatives are available*. Although process synthesis is enjoyable as a creative activity, the industrial practice of process design is usually more concerned with delivering designs that will work reliably and quickly make money to generate a return on investment. Successful companies are usually good at focusing the creativity of their employees on critical areas where innovation can provide a competitive advantage, without turning every project into an open-ended research problem.

TABLE 2.2 Sample questions that can be asked in a PFD review

Process Section	Questions
Feed preparation	How is (each) feed delivered?
	How is (each) feed stored?
	How much inventory of (each) feed is required?
	How is feed transferred from storage to the process?
	How is the rate of feed supply controlled?
	Is any feed pretreatment necessary before the feed is sent to the process?
	For solid feeds, is any feed size adjustment necessary?
	Is any heating or cooling needed before the feed is sent to the process?
Reaction	What are the reacting species?
	What side reactions occur?
	What are the reaction conditions and why were they chosen?
	How are the reaction conditions maintained or controlled?
	How are inventories of solids, liquid, or vapor in the reactor controlled?
	What are the reactor design specifications (e.g., residence time, interfacial area)?
	What are the estimated reactor yield and selectivity?
	What reactor type was chosen and why was it selected?
	Is a catalyst used? If so, is the catalyst stable or does it require periodic regeneration?
	Is heat addition or removal necessary?
	Are there specific safety issues that should be considered?
	(Additional information on reactor design is given in Chapter 15, which may prompt more questions)
Product Recovery	What is the purpose of each separation?
	What are the process conditions (temperature, pressure, etc.)?
	What are the equipment specifications (recovery, purity, etc.)?
	Why was a particular separation selected?
	Is heat removal or addition necessary?
	Can heat addition or removal be accomplished by process-to-process heat transfer?
	How are inventories of vapor, liquid, or solid controlled in each operation?
	How is the operation controlled to achieve the desired specifications?
	Are there specific safety issues that should be considered?
Purification	What are the final product specifications?
	What are the specifications for any by-products?
	What are the specifications for any effluents discharged to the environment?
	What are the specifications for any recycle streams returned to the process?
	What are the specifications for any waste streams sent to disposal?
	How are final purity specifications on any stream leaving the process achieved?
	How is the process controlled to ensure that purity specifications can be achieved?

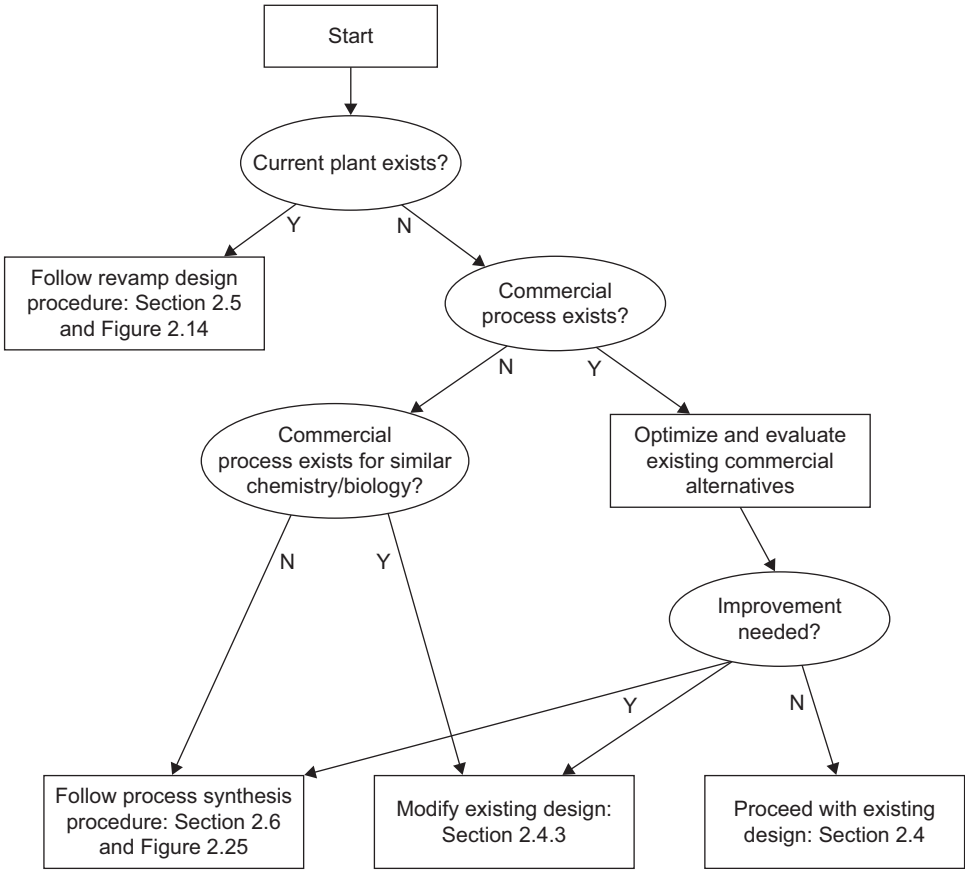


FIG. 2.30 Overall procedure for flowsheet development.

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2.10 Nomenclature

		Dimensions in MLT
A	Area for heat exchange	$\mathbf{L}^2$
$C_{p,f}$	Specific heat capacity of feed	$\mathbf{L^2T^{-2}\theta^{-1}}$
$C_{p,i}$	Specific heat capacity of stream i	$\mathbf{L^2T^{-2}\theta^{-1}}$
$C_{p,p}$	Specific heat capacity of product	$\mathbf{L^2T^{-2}\theta^{-1}}$
F	Unknown flow, Example 2.6	$\mathbf{MT^{-1}}$
F_{cw}	Flow rate of cooling water	$\mathbf{MT^{-1}}$
F_t	Log mean temperature difference correction factor (see Chapter 19)	—
m_f	Mass flow rate of feed	$\mathbf{MT^{-1}}$
m_i	Mass flow rate of stream i	$\mathbf{MT^{-1}}$
m_p	Mass flow rate of product	$\mathbf{MT^{-1}}$
Q	Rate of heat transfer	$\mathbf{ML^2T^{-3}}$
SV	Space velocity	$\mathbf{T^{-1}}$
T_1	Unknown temperature, Example 2.7	$\boldsymbol{\theta}$
T_2	Unknown temperature, Example 2.7	$\boldsymbol{\theta}$
T_3	Unknown temperature, Example 2.7	$\boldsymbol{\theta}$
T_s	Steam temperature	$\boldsymbol{\theta}$
T_w	Cooling water outlet temperature	$\boldsymbol{\theta}$
ΔT_i	Change in temperature of stream i for a stream undergoing sensible heat changes	$\boldsymbol{\theta}$
ΔT_{lm}	Logarithmic mean temperature difference	$\boldsymbol{\theta}$
ΔT_m	Mean temperature difference for heat transfer	$\boldsymbol{\theta}$
U	Overall heat transfer coefficient	$\mathbf{MT^{-3}\theta^{-1}}$
V	Reactor volume	$\mathbf{L}^3$
V_{cat}	Catalyst fixed bed volume	$\mathbf{L}^3$
v	Volumetric flow rate	$\mathbf{L^3T^{-1}}$
X	Unknown flow, Examples 2.1, 2.5	$\mathbf{MT^{-1}}$
Y	Unknown flow, Example 2.5	$\mathbf{MT^{-1}}$
Z	Unknown flow, Example 2.5	$\mathbf{MT^{-1}}$
τ	Residence time	$\mathbf{T}$

Common PFD abbreviations

BFW Boiler feed water
CW Cooling water
CTW Cooling tower water
DBO Design by others (used to refer to a section of a flowsheet that is purchased from a vendor as a packaged plant)
DIW Deionized water
HPS High-pressure steam
LPS Low-pressure steam
MPS Medium-pressure steam
NNF Normally no flow (used to indicate discontinuous operations in a continuous plant flowsheet)
ROW Reverse-osmosis water

Abbreviations for designating process control instruments are given in Chapter 5.

2.11 Problems

2.1. Cinnamic aldehyde (a fragrance compound) can be made by base-catalyzed aldol condensation reaction between benzaldehyde and acetaldehyde. The feeds are contacted with sodium hydroxide in a stirred tank reactor. The product is neutralized and washed with water to remove salts. The washed product is usually separated by batch distillation, in which unreacted feeds are recovered first, followed by product, and a polymeric waste is left as residue. The batch distillation product can be further purified by vacuum distillation. Sketch a block flow diagram of the process.

2.2. Cumene is made by alkylation of benzene with propylene over zeolitic catalyst. To maximize selectivity to desired products, several beds of catalyst are used inside the same reactor. A mixture of feed and recycle benzene enters the top of the reactor and the feed propylene is split so that a portion of the propylene is fed to each catalyst bed. A large excess of benzene is used to minimize propylene oligomerization and ensure complete reaction of propylene. The reactor product is cooled and sent to a stabilizer column that removes any light hydrocarbons. The bottoms from this column are sent to a benzene column that recovers benzene overhead for recycle to the alkylation and transalkylation reactors. The bottoms from the benzene column are distilled to give cumene product and a heavy stream. The heavy stream is further distilled in a heavies column to give a mixture of dipropyl- and tripropyl-benzene overhead and a heavy waste stream as bottoms. The distillate from the heavies column is sent to a transalkylation reactor and reacted with excess benzene. The product from the transalkylation reactor is returned to the benzene column. Sketch a block flow diagram of the process.

2.3. Cyclosporin A is produced by fermentation using either *Cylindrocarpon lucidum* Booth or *Tolypocladium inflatum* Gams. The fermentation is carried out in batch reactors, which are filled with a feed medium, inoculated with the fungi, and aerated for a period of 13 days. The reactor product is milled and extracted with 90% methanol. The methanol is evaporated off to give an aqueous solution that is then extracted with ethylene chloride. The organic solution is evaporated to dryness, and then the product is purified by chromatography in methanol over aluminum oxide or silica gel. Sketch a block flow diagram of the process.

2.4. The composition of a gas derived by the gasification of coal is volume percentage: carbon dioxide 4, carbon monoxide 16, hydrogen 50, methane 15, ethane 3, benzene 2, balance nitrogen. If the gas is burnt in a furnace with 20% excess air, calculate:

a. The amount of air required per 100 kmol of gas
b. The amount of flue gas produced per 100 kmol of gas
c. The composition of the flue gases, on a dry basis

Assume complete combustion.

2.5. The off-gases from a gasoline stabilizer are fed to a steam reforming plant to produce hydrogen. The composition of the off-gas, molar%, is CH_4 77.5, C_2H_6 9.5, C_3H_8 8.5, C_4H_{10} 4.5. The gases entering the reformer are at a pressure of 2 bara and 35 °C and the feed rate is 2000 m^3/h.

The reactions in the reformer are:

$$1.\ C_2H_{2n+1} + n(H_2O) \rightarrow n(CO) + (2_n + 1)H_2$$

$$2.\ CO + H_2O \rightarrow CO_2 + H_2$$

The molar conversion of C_2H_{2n+2} in reaction (1) is 96% and of CO in reaction (2) is 92%.
Calculate:

a. The average molecular mass of the off-gas
b. The mass of gas fed to the reformer, kg/h
c. The mass of hydrogen produced, kg/h

2.6. Allyl alcohol can be produced by the hydrolysis of allyl chloride. Together with the main product, allyl alcohol, di-allyl ether is produced as a by-product. The conversion of allyl chloride is typically 97% and the selectivity to alcohol is 90%, both on a molar basis. Assuming that there are no other significant side reactions, calculate masses of alcohol and ether produced per 1000 kg of allyl chloride fed to the reactor.

2.7. Aniline is produced by the hydrogenation of nitrobenzene. A small amount of cyclo-hexylamine is produced as a by-product. The reactions are:

$$1.\ C_2H_5NO_2 + 3H_2 \rightarrow C_6H_5NH_2 + 2H_2O$$

$$2.\ C_6H_5NO_2 + 6H_2 \rightarrow C_6H_{11}NH_2 + 2H_2O$$

Nitrobenzene is fed to the reactor as a vapor, with three times the stoichiometric quantity of hydrogen. The conversion of the nitrobenzene to all products is 96%, and the selectivity for aniline is 95%.
The unreacted hydrogen is separated from the reactor products and recycled to the reactor. A purge is taken from the recycle stream to maintain the inerts in the recycle stream below 5%. The fresh hydrogen feed is 99.5% pure, with the remainder being inerts. All percentages are molar.
For a feed rate of 100 kmol/h of nitrobenzene, calculate:

a. The fresh hydrogen feed
b. The purge rate required
c. The composition of the reactor outlet stream

2.8. Guaifenesin [guaiacol glyceryl ether, 3-(2-methoxyphenoxy)-1,2-propanediol, $C_{10}H_{14}O_4$] is an expectorant that is found in cough medicines such as Actifed and Robitussin. U.S. Patent 4,390,732 (to Degussa) describes a preparation of the active pharmaceutical ingredient (API) from guaiacol (2-methoxyphenol, $C_7H_8O_2$) and glycidol (3-hydroxy propylene oxide, $C_3H_6O_2$). When the reaction is catalyzed by NaOH, the reaction yield is 93.8%. The product is purified in a thin-film evaporator, giving an overall plant yield of 87%.
a. Estimate the feed flow rates of glycidol and guaiacol that would be needed to produce 100 kg/day of the API.
b. Estimate how much product is lost in the thin-film evaporator.
c. How would you recover the product lost in the evaporator?

2.9. 11-[N-ethoxycarbonyl-4-piperidylidene]-8-chloro-6,11-dihydro-5H-benzo-[5,6]-cyclohepta-[1,2-b]-pyridine ($C_{22}H_{23}ClN_2O_2$) is a nonsedative antihistamine known as loratadine and marketed as Claritin The preparation of the API is described in U.S. Patent 4,282,233 (to Schering). The patent describes reacting 16.2g of 11-[N-methyl-4-piperidylidene]-8-chloro-6,11-dihydro-5H-benzo-[5,6]-cyclohepta-[1,2-b]-pyridine ($C_{20}H_{21}ClN_2$) in 200 mL of benzene with 10.9 g of ethylchloroformate ($C_3H_5ClO_2$) for 18 hours. The mixture is cooled, poured into ice water, and separated into aqueous and organic phases. The organic layer is washed with water and evaporated to dryness. The residue is triturated (ground to a fine powder) with petroleum ether and recrystallized from isopropyl ether.
a. What is the reaction by-product?
b. The reaction appears to be carried out under conditions that maximize both selectivity and conversion (long time at low temperature), as might be expected given the cost of the raw material. If the conversion is 99.9% and the selectivity for the desired ethoxycarbonyl substituted compound is 100%, how much excess ethylchloroformate remains at the end of the reaction?

c. What fraction of the ethylchloroformate feed is lost to waste products?
d. Assuming that the volumes of water and isopropyl ether used in the quenching, washing, and recrystallization steps are the same as the initial solvent volume and that none of these materials are reused in the process, estimate the total mass of waste material produced per kg of the API.
e. If the recovery (plant yield) of the API from the washing and recrystallization steps is 92%, estimate the feed flow rates of 11-[N-methyl-4-piperidylidene]-8-chloro-6,11-dihydro-5H-benzo-[5,6]-cyclohepta-[1,2-b]-pyridine and ethylchloroformate required to produce a batch of 10 kg of the API.
f. How much API could be produced per batch in a 3.8 m^3 (1000 U.S. gal) reactor?
g. What would be the advantages and disadvantages of carrying out the other process steps in the same vessel?
h. Sketch a block flow diagram of the process.

2.10. Describe the main commercial process used to make each of the following compounds. Include a block flow diagram.
a. Phosphoric acid
b. Adipic acid
c. Polyethylene terephthalate
d. Insulin
e. Sorbitol

2.11. Example 2.7 introduced a heat-exchange system revamp problem. If the plate heat exchanger E101 in Fig. 2.19 is the gasketed-plate type, then the exchanger area can be increased by adding plates to the exchanger. How much additional area must be added to E101 to allow the system to operate at 50% above base case flow rate with no changes in temperature of steam or cooling water feed temperatures and no modification to exchangers E102 and E103?

2.12. Styrene is made by dehydrogenation of ethylbenzene, which is formed by alkylation of benzene with ethylene. Propose target yields for the alkylation and dehydrogenation steps if the forecasted prices per metric ton are styrene $800, ethylene $800, and benzene $500.

Note: Structures for the compounds in Problems 2.3, 2.8, and 2.9 can be found in the Merck Index, but are not required to solve the problems.

CHAPTER

3

Utilities and energy-efficient design

KEY LEARNING OBJECTIVES

- How processes are heated and cooled
- The systems used for delivering steam, cooling water, and other site utilities
- Methods used for recovering process waste heat
- How to use the pinch design method to optimize process heat recovery
- How to design a heat-exchanger network
- How energy is managed in batch processes

3.1 Introduction

Very few chemical processes are carried out entirely at ambient temperature. Most require process streams to be heated or cooled to reach the desired operation temperature; to add or remove heats of reaction, mixing, adsorption, etc.; to sterilize feed streams; or to cause vaporization or condensation. Gas and liquid streams are usually heated or cooled by indirect heat exchange with another fluid: either another process stream or a utility stream such as steam, hot oil, cooling water, or refrigerant. The design of heat exchange equipment for fluids is addressed in Chapter 19. Solids are usually heated and cooled by direct heat transfer, as described in Chapter 18. This chapter begins with a discussion of the different utilities that are used for heating, cooling, and supplying other needs such as power, water, and air to a process.

The consumption of energy is a significant cost in many processes. Energy costs can be reduced by recovering waste heat from hot process streams and by making use of the fuel value of waste streams. Section 3.4 discusses how to evaluate waste stream combustion as a source of process heat. Section 3.3 introduces other heat recovery approaches.

When it is economically attractive, heating and cooling are accomplished by heat recovery between process streams. The design of a network of heat exchangers for heat recovery can be a complex task if there are many hot and cold streams in a process. Pinch analysis, introduced in Section 3.5, is a systematic method for simplifying this problem.

The efficient use of energy in batch and cyclic processes is made more complicated by the sequential nature of process operations. Some approaches to energy-efficient design of batch and cyclic processes are discussed in Section 3.6.

3.2 Utilities

The word *utilities* is used for the ancillary services needed in the operation of any production process. These services are normally supplied from a central site facility and include:

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1. Electricity
2. Fuel for fired heaters
3. Fluids for process heating
   a. Steam
   b. Hot oil or specialized heat transfer fluids
4. Fluids for process cooling
   a. Cooling water
   b. Chilled water
   c. Refrigeration systems
5. Process water
   a. Water for general use
   b. Demineralized water
6. Compressed air
7. Inert-gas supplies (usually nitrogen)

Most plants are located on sites where the utilities are provided by the site infrastructure. The price charged for a utility is mainly determined by the operating cost of generating and transmitting the utility stream. Some companies also include a capital recovery charge in the utility cost, but if this is done, then the offsite (OSBL) capital cost of projects must be reduced to avoid double counting and biasing the project capital–energy trade-off, leading to poor use of capital.

Some smaller plants purchase utilities "over the fence" from a supplier, such as a larger site or a utility company, in which case the utility prices are set by contract and are typically pegged to the price of natural gas, fuel oil, or electricity.

The utility consumption of a process cannot be estimated accurately without completing the material and energy balances and carrying out a pinch analysis, as described in Section 3.5.6. The pinch analysis gives targets for process heat recovery and hence for the minimum requirements of hot and cold utilities. More detailed optimization then translates these targets into expected demands for fired heat, steam, electricity, cooling water, and refrigeration. In addition to the utilities required for heating and cooling, the process may need process water and air for applications such as washing, stripping, and instrument air supply. Good overviews of methods for design and optimization of utility systems are given by Smith (2016), Knopf (2012), Zhu (2014), and Kemp (2007).

3.2.1 Electricity

The electricity demand of the process is mainly determined by the work required for pumping, compression, air coolers, and solids-handling operations, but also includes the power needed for instruments, lights, and other small users. The power required may be generated on site, but will more usually be purchased from the local supply company. Some plants generate their own electricity using a gas-turbine cogeneration plant with a heat recovery steam generator (waste heat boiler) to raise steam (Fig. 3.1). The overall thermal efficiency of such systems can be

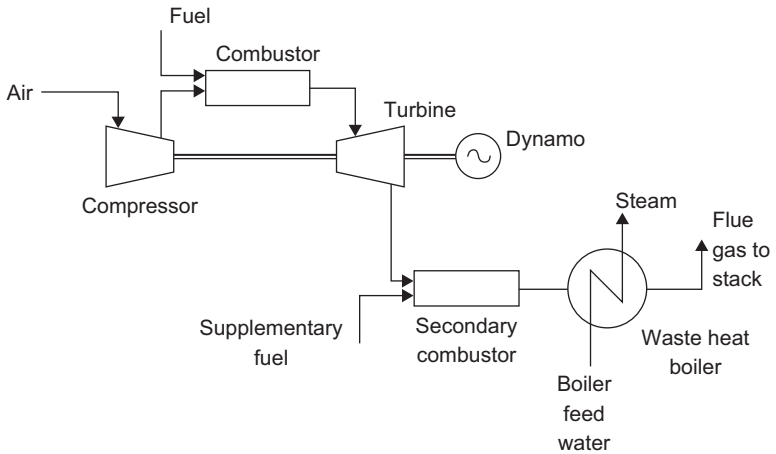


Fig. 3.1 Gas turbine–based cogeneration plant.

in the range of 70% to 80%, compared with the 30% to 40% obtained from a conventional power station, where the heat in the exhaust steam is wasted in the condenser. The cogeneration plant can be sized to meet or exceed the plant electricity requirement, depending on whether the export of electricity is an attractive use of capital. This "make or buy" scenario gives chemical producers strong leverage when negotiating electric power contracts, and they are usually able to purchase electricity at or close to wholesale prices. Wholesale electricity prices vary regionally (see www.eia.gov for details), but are typically about $0.06/kWh in North America at the time of writing.

The voltage at which the supply is taken or generated will depend on the demand. In the United States, power is 135, 220, 550, or 750 kV. Local substations step the power down to 35 to 69 kV for medium-voltage transmission and then to 4 to 15 kV local distribution lines. Transformers at the plant are used to step down the power to the supply voltages used on site. Most motors and other process equipment run on 208 V three-phase power, whereas 120/240 V single-phase power is used for offices, labs, and control rooms.

On any site it is always worth considering driving large compressors and pumps with steam turbines instead of electric motors and using the exhaust steam for local process heating.

Electric power is rarely used for heating in large-scale chemical plants, although it is often used in smaller batch processes that handle nonflammable materials, such as biological processes. The main disadvantages of electrical heating for large-scale processes are:

- Heat from electricity is typically two to three times more expensive than heat from fuels because of the thermodynamic inefficiency of power generation.
- Electric heating requires very high power draws that would substantially increase the electrical infrastructure costs of the site.
- Electric heating apparatus is expensive, requires high maintenance, and must comply with stringent safety requirements when used in areas where flammable materials may be present.
- Electric heaters are intrinsically less safe than steam systems. The maximum temperature that a steam heater can reach is the temperature of the steam. The maximum temperature of an electric heater is determined by the temperature controller (which could fail) or by burnout of the heating element. Electric heaters therefore have a higher probability of overheating.

Electric heating is more likely to be attractive in small-scale batch or cyclic processes, particularly when the cost of heating is a small fraction of overall process costs and when the process calls for rapid on-off heating.

A detailed account of the factors to be considered when designing electrical distribution systems for chemical process plants and the equipment used (transformers, switch gear, and cables) is given by Silverman (1964). Requirements for electrical equipment used in hazardous (classified) locations are given in the National Electrical Code (NFPA 70), as described in Section 10.3.5.

3.2.2 Fired heat

Fired heaters are used for process heating duties above the highest temperatures that can be reached using high-pressure steam, typically about 250 °C (482 °F). Process streams may be heated directly in the furnace tubes or indirectly using a hot oil circuit or heat transfer fluid, as described in Section 3.2.4. The design of fired heaters is described in Section 19.17. The cost of fired heat can be calculated from the price of the fuel fired. Most fired process heaters use natural gas as fuel, as it is cleaner burning than fuel oil and therefore easier to fit NO_x control systems and obtain permits. Natural gas also requires less maintenance of burners and fuel lines, and natural gas burners can often cofire process waste streams, such as hydrogen, light organic compounds, or air saturated with organic compounds.

Natural gas and heating oil are traded as commodities, and prices can be found at any online trading site or business news site (e.g.,www.cnn.com/business). Historic prices for forecasting can be found in the *Oil and Gas Journal* or from the U.S. Energy Information Agency (www.eia.gov).

The fuel consumed in a fired heater can be estimated from the fired heater duty divided by the furnace efficiency. The furnace efficiency will typically be about 0.85 if both the radiant and convective sections are used (see Chapter 19) and about 0.6 if the process heating is in the radiant section only.

Example 3.1

Estimate the annual cost of providing heat to a process from a fired heater using natural gas as fuel if the process duty is 4 MW and the price of natural gas is $3.20/MMBtu (million Btu).

Solution

If we assume that the fired heater uses both the radiant and convective sections, then we can start by assuming a heater efficiency of 0.85, so:

$$\text{Fuel required} = \text{Heater duty} \;/\; \text{heater efficiency} = 4/0.85 = 4.71 \text{ MW}$$

$$1 \text{ Btu/h} = 0.29307 \text{ W, so } 4.71 \text{ MW} = 4.71/0.29307 = 16.07 \text{ MMBtu/h}$$

Assuming 8000 operating hours per year, the total annual fuel consumption would be:

$$\text{Annual fuel use} = 16.07 \times 8000 = 128.6 \times 10^3 \text{ MMBtu}$$

$$\text{Annual cost of fired heat} = 128.6 \times 10^3 \times 3.20 = \$411{,}400$$

Note that if we had decided to carry out all of the heating in the radiant section only, then the fuel required would have been 4 / 0.6 = 6.67 MW and the annual cost of heating would increase to $582,600 unless we could find some other process use for the heat available in the convective section of the heater.

3.2.3 Steam

Steam is the most widely used heat source in most chemical plants. Steam has a number of advantages as a hot utility:

- The heat of condensation of steam is high, giving a high heat output per pound of utility at constant temperature (compared with other utilities such as hot oil and flue gas that release sensible heat over a broad temperature range).
- The temperature at which heat is released can be precisely controlled by controlling the pressure of the steam. This enables tight temperature control, which is important in many processes.
- Condensing steam has very high heat transfer coefficients, leading to cheaper heat exchangers.
- Steam is nontoxic, nonflammable, visible if it leaks externally and inert to many (but not all) process fluids.

Most sites have a pipe network supplying steam at three or more pressure levels for different process uses. A typical steam system is illustrated in Fig. 3.2. Boiler feed water (BFW) at high pressure is preheated and fed to boilers, where high-pressure (HP) steam is raised and superheated above the dew point to allow for heat losses in the piping. Boiler feed water preheat can be accomplished using process waste heat or convective section heating in the boiler plant. HP steam is typically at about 40 bar, corresponding to a condensing temperature of 250 °C, but every site is different. Some of the HP steam is used for process heating at high temperatures. The remainder of the HP steam is expanded either through let-down valves or steam turbines known as *back-pressure turbines* to form

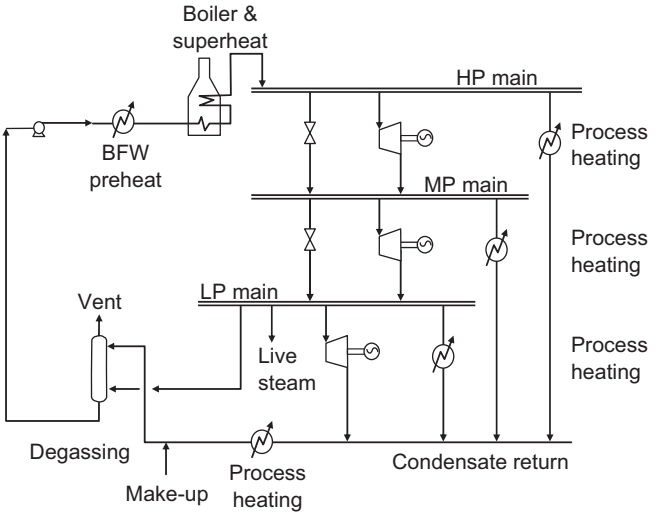


Fig. 3.2 Steam system.

medium-pressure (MP) steam. The pressure of the MP steam mains varies widely from site to site, but is typically about 20 bar, corresponding to a condensing temperature of 212 °C. MP steam is used for intermediate-temperature heating or expanded to form low-pressure (LP) steam, typically at about 3 bar, condensing at 134 °C. Some of the LP steam may be used for process heating if there are low-temperature heat requirements. LP (or MP or HP) steam can also be expanded in condensing turbines to generate shaft work for process drives or electricity production. A small amount of LP steam is used to strip dissolved noncondensable gases such as air from the condensate and make-up water. LP steam is also often used as "live steam" in the process, for example, as stripping vapor or for cleaning, purging, or sterilizing equipment.

When steam is condensed without coming into contact with process fluids, the hot condensate can be collected and returned to the boiler feed water system. Condensate can also sometimes be used as a low-temperature heat source if the process requires low-temperature heat.

The price of HP steam can be estimated from the cost of boiler feed water treatment, the price of fuel, and the boiler efficiency:

$$P_{HPS} = P_F \times \frac{dH_b}{\eta_B} + P_{BFW} \tag{3.1}$$

where: P_{HPS} = price of HP steam ($/1000 lb, commonly written $/Mlb)
P_F = price of fuel ($/MMBtu)
dH_b = heating rate (MMBtu/Mlb steam)
η_B = boiler efficiency
P_{BFW} = price or cost of boiler feed water ($/Mlb)

Package boilers typically have efficiencies similar to fired heaters, in the range of 0.8 to 0.9. The heating rate should include boiler feed water preheat, the latent heat of vaporization, and the superheat specified. The steam for process heating is usually generated in water-tube boilers, using the most economical fuel available.

The cost of boiler feed water includes allowances for water make-up, chemical treatment, and degassing, and is typically about twice the cost of raw water (see later). If no information on the price of water is available, then 0.50 $/1000 lb can be used as an initial estimate. If the steam is condensed and the condensate is returned to the boiler feed water (which will normally be the case), then the price of steam should include a credit for the condensate. The condensate credit will often be close enough to the boiler feed water cost that the two terms cancel each other out and can be neglected.

The prices of MP and LP steam are usually discounted from the HP steam price to allow for the shaft work credit that can be gained by expanding the steam through a turbine and also to encourage process heat recovery by raising steam at intermediate levels and using low-grade heat when possible. Several methods of discounting are used. The most rational of these is to calculate the shaft work generated by expanding the steam between levels and price this as equivalent to electricity (which could be generated by attaching the turbine to a dynamo or else would be needed to run a motor to replace the turbine if it is used as a driver). The value of the shaft work then sets the discount between steam at different levels. This is illustrated in the following example.

Example 3.2

A site has steam levels at 40 bar, 20 bar, and 6 bar. The price of fuel is $6/MMBtu, and electricity costs $0.05/kWh. If the boiler efficiency is 0.8 and the steam turbine efficiency is 0.85, suggest prices for HP, MP, and LP steam.

Solution

The first step is to look up the steam conditions, enthalpies, and entropies in steam tables:

Steam level	HP	MP	LP
Pressure (bar)	40	20	6
Saturation temperature (°C)	250	212	159

The steam will be superheated above the saturation temperature to allow for heat losses in the pipe network. The following superheat temperatures were set to give an adequate margin above the saturation temperature for HP steam and also to give (roughly) the same specific entropy for each steam level. The actual superheat temperatures of MP and LP steam will be higher due to the nonisentropic nature of the expansion.

Superheat temperature (°C)	400	300	160
Specific entropy, sg, (kJ/kg.K)	6.769	6.768	6.761
Specific enthalpy, hg, (kJ/kg)	3214	3025	2757

We can then calculate the difference in enthalpy between levels for isentropic expansion:

Isentropic delta enthalpy (kJ/kg)	189	268

Multiplying by the turbine efficiency gives the nonisentropic enthalpy of expansion:

Actual delta enthalpy (kJ/kg)	161	228

This can be converted to give the shaft work in customary units:

Shaft work (kWh/Mlb)	20.2	28.7

Multiplying by the price of electricity converts this into a shaft work credit:

Shaft work credit ($/Mlb)	1.01	1.44

The price of HP steam can be found from Equation 3.1, assuming that the boiler feed water cost is cancelled out by a condensate credit. The other prices can then be estimated by subtracting the shaft work credits.

Steam price ($/Mlb)	6.48	5.47	4.03

For quick estimates, this example can easily be coded into a spreadsheet and updated with the current prices of fuel and power. A sample steam-costing spreadsheet is available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

3.2.4 Hot oil and heat transfer fluids

Circulating systems of hot oil or specialized heat transfer fluids are often used as heat sources in situations where fired heat or steam is not suitable. Heat transfer fluids and mineral oils can be used over a temperature range from 50 °C to 400 °C. The upper temperature limit on use of hot oils is usually set by thermal decomposition of the oil, fouling, or coking of heat-exchange tubes. Some heat transfer fluids are designed to be vaporized and condensed in a similar manner to the steam system, though at lower pressures; however, vaporization of mineral oils is usually avoided, as less volatile components in the oil could accumulate and decompose, causing accelerated fouling.

The most common situation where a hot oil system is used is in plants that have many relatively small high-temperature heating requirements. Instead of building several small fired heaters, it can be more economical to supply heat to the process from circulating hot oil streams and build a single fired heater that heats the hot oil. Use of hot oil also reduces the risk of process streams being exposed to high tube-wall temperatures that might be experienced in a fired heater. Hot oil systems are often attractive when there is an HP differential between the process stream and HP steam and use of steam would entail using thicker tubes. Hot oil systems can sometimes be justified on safety grounds if the possibility of steam leakage into the process is hazardous.

The most commonly used heat transfer fluids are mineral oils and Dowtherm A. Mineral oil systems usually require large flow rates of circulating liquid oil. When the oil is taken from a process stream, as is common in oil refining processes, then it is sometimes called a *pump-around system*. Dowtherm A is a mixture of 26.5 wt% diphenyl in diphenyl oxide. Dowtherm A is thermally stable and is usually operated in a vaporization−condensation cycle similar to the steam system, although condensed liquid Dowtherm is sometimes used for intermediate-temperature heating requirements. The design of Dowtherm systems and other proprietary heat transfer fluids is discussed in detail in Singh (1985) and Green and Southard (2018).

The cost of the initial charge of heat transfer fluid usually makes a negligible contribution to the overall cost of running a hot oil system. The main operating cost is the cost of providing heat to the hot oil in the fired heater or

vaporizer. If a pumped liquid system is used, then the pumping costs should also be evaluated. The costs of providing fired heat are discussed in Section 3.2.2. Hot oil heaters or vaporizers usually use both the radiant and convective sections of the heater and have heater efficiencies in the range 80% to 85%.

3.2.5 Cooling water

When a process stream requires cooling at high temperature, various heat recovery techniques should be considered. These include transferring heat to a cooler process stream, raising steam, preheating boiler feed water, etc., as discussed in Section 3.3.

When heat must be rejected at lower temperatures, below about 120 °C (248 °F) (more strictly, below the pinch temperature), then a cold utility stream is needed. Cooling water is the most commonly used cold utility in the temperature range of 120 °C to 40 °C, although air cooling is preferred in regions where water is expensive or the ambient humidity is too high for cooling water systems to operate effectively. The selection and design of air coolers are discussed in Section 19.16. If a process stream must be cooled to a temperature below 40 °C, cooling water or air cooling would be used down to a temperature in the range 40° to 50 °C, followed by chilled water or refrigeration down to the target temperature.

Natural and forced-draft cooling towers are generally used to provide the cooling water required on a site unless water can be drawn from a convenient river or lake in sufficient quantity. Sea water or brackish water can be used at coastal sites and for offshore operations, but if used directly will require the use of more expensive materials of construction for heat exchangers (see Chapter 6). The minimum temperature that can be reached with cooling water depends on the local climate. Cooling towers work by evaporating part of the circulating water to ambient air, causing the remaining water to be chilled. If the ambient temperature and humidity are high, then a cooling water system will be less effective, and air coolers or refrigeration would be used instead.

A schematic of a cooling water system is shown in Fig. 3.3. Cooling water is pumped from the cooling tower to provide coolant for the various process cooling duties. Each process cooler is served in parallel, and cooling water almost never flows to two coolers in series. The warmed water is returned to the cooling tower and cooled by partial evaporation. A purge stream known as a *blowdown* is removed upstream of the cooling tower to prevent the accumulation of dissolved solids as water evaporates from the system. A make-up stream is added to compensate for evaporative losses, blowdown losses, and any other losses from the system. Small amounts of chemical additives are also usually fed into the cooling water to act as biocides and corrosion and fouling inhibitors.

The cooling tower consists of a means of providing high surface area for heat and mass transfer between the warm water and ambient air and a means of causing air to flow counter-current to the water. The surface area for contact is usually provided by flowing the water over wooden slats or high-voidage packing. The cooled water is then collected at the bottom of the tower. In most modern cooling towers the air flow is induced by fans that are placed above the packed section of the tower. For very large cooling loads natural-draft cooling towers are used, in which a large hyperbolic chimney is placed above the packed section to induce air flow. Some older plants use spray ponds instead of cooling towers.

Cooling water systems can be designed using a psychrometric chart if the ambient conditions are known. A psychrometric chart is given in Fig. 3.4. The cooling tower is usually designed so that it will operate effectively except under the hottest (or most humid) conditions that can be expected to occur no more than a few days each year.

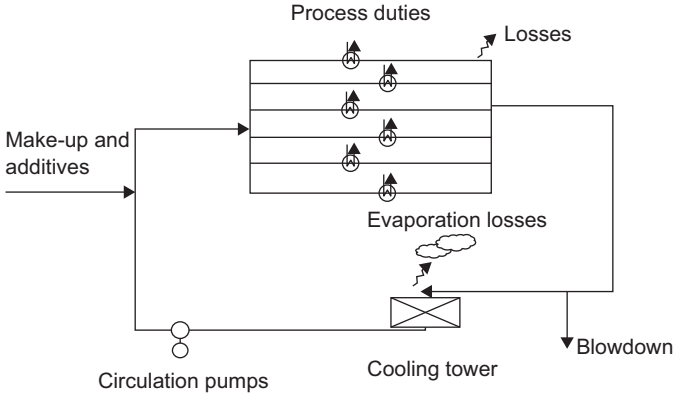


Fig. 3.3 Schematic of cooling water system.

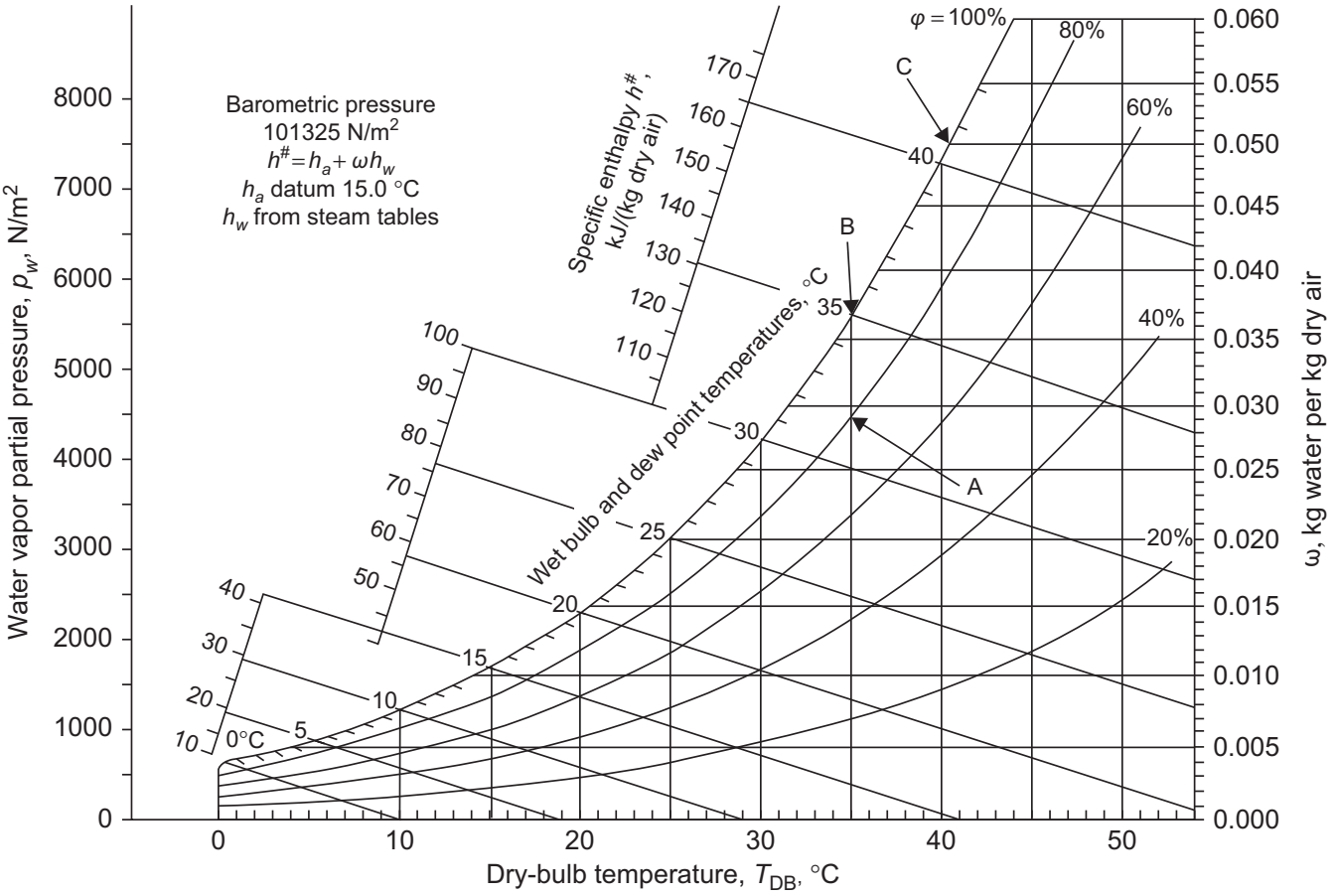


Fig. 3.4 Psychrometric chart. *Adapted with permission from Balmer, R. [2010]. Thermodynamic tables to accompany modern engineering thermodynamics [Academic Press].*

The ambient temperature and humidity can be plotted on the psychrometric chart, allowing the inlet air wet bulb temperature to be determined. This is the coldest temperature that the cooling water could theoretically reach; however, in practice most cooling towers operate with a temperature approach to the air wet bulb temperature of at least 2.8 °C (5 °F). Adding the approach temperature to the inlet air wet bulb temperature, we can then mark the outlet water condition on the saturation curve. For example, if the hottest ambient condition for design purposes is a dry bulb temperature of 35 °C (95 °F) with 80% humidity, then we can mark this point on the psychrometric chart (point A) and read the wet bulb temperature as roughly 32 °C (89.6 °F). Adding a 2.8 °C temperature approach would give a cold water temperature of about 35 °C (95 °F), which can then be marked on the saturation line (point B).

The inlet water condition, or cooling water return temperature, is found by optimizing the trade-off between water circulation costs and cooling tower cost. The difference between the cooling water supply (coldest) and return (hottest) temperatures is known as the *range* or *cooling range* of the cooling tower. As the cooling range increases, the cost of the cooling tower increases, but the water flow rate that must be circulated decreases, and hence the pumping cost decreases. Note that because most of the cooling is accomplished by evaporation of water rather than transfer of sensible heat to the air, the evaporative losses do not vary much with the cooling range. Most cooling towers are operated with a cooling range between 2.8° to 11.1 °C (5° and 20 °F). A typical initial design point would be to assume a cooling water return temperature about 5.5 °C (10 °F) hotter than the cold water temperature. In the example earlier, this would give a cooling water return temperature of 40.5 °C (105 °F), which can also be marked on the psychrometric chart (point C). The difference in air humidity across the cooling tower can now be read from the right-hand axis as the difference in moisture loadings between the inlet air (point A) and the outlet air (point C). The cooling tower design can then be completed by determining the cooling load of the water from an energy balance and hence determining the flow rate of air that is needed based on the change in air humidity between ambient air and the air exit condition. The exit air is assumed to have a dry bulb temperature equal to the cooling water return temperature, and the minimum air flow will be obtained when the air leaves saturated with moisture. Examples of the detailed design of cooling towers are given in Green and Southard (2018).

When carrying out the detailed design of a cooling tower, it is important to check that the cooling system has sufficient capacity to meet the site cooling needs over a range of ambient conditions. In practice, multiple cooling water pumps are usually used so that a wide range of cooling water flow rates can be achieved. When new capacity is added to an existing site, the limit on the cooling system is usually the capacity of the cooling tower. If the cooling tower fans cannot be upgraded to meet the increased cooling duty, additional cooling towers must be added. In such cases, it is often cheaper to install air coolers for the new process rather than upgrading the cooling water system.

The cost of providing cooling water is mainly determined by the cost of electric power. Cooling water systems use power for pumping the cooling water through the system and for running fans (if installed) in the cooling towers. They also have costs for water make-up and chemical treatment. The power used in a typical recirculating cooling water system is usually between 1 and 2 kWh/1000 gal of circulating water. The costs of water make-up and chemical treatment usually add about $0.02/1000 gal.

3.2.6 Refrigeration

Refrigeration is needed for processes that require temperatures below those that can be economically obtained with cooling water (i.e., below about 40 °C). For temperatures down to around 10 °C, chilled water can be used. For lower temperatures, down to −30 °C, salt brines (NaCl and $CaCl_2$) are sometimes used to distribute the "refrigeration" around the site from a central refrigeration machine. Large refrigeration duties are usually supplied by a stand-alone packaged refrigeration system.

Vapor compression refrigeration machines are normally used, as illustrated in Fig. 3.5. The working fluid (refrigerant) is compressed as a vapor and then cooled and condensed at HP, allowing heat rejection at high temperature in an exchanger known as a *condenser*. Heat is usually rejected to a coolant such as cooling water or ambient air. The liquid refrigerant is then expanded across a valve to a lower pressure, where it is vaporized in an exchanger known as an *evaporator*, taking up heat at low temperature. The vapor is then returned to the compressor, completing the cycle.

The working fluid for a refrigeration system must satisfy a broad range of requirements. It should have a boiling point that is colder than the temperature that must be reached in the process at a pressure that is above atmospheric pressure (to prevent leaks into the system). It should have a high latent heat of evaporation to reduce refrigerant flow rate. The system should operate well below the critical temperature and pressure of the refrigerant, and the condenser pressure should not be too high or the cost will be excessive. The freezing temperature of the refrigerant must be well below the minimum operating temperature of the system. The refrigerant should also be nontoxic, nonflammable, and have minimal environmental impact.

A wide range of materials have been developed for use as refrigerants, most of which are halogenated hydrocarbons. In some situations ammonia, nitrogen, and carbon dioxide are used. Cryogenic gas separation processes usually use the process fluids as working fluid; for example, ethylene and propylene refrigeration cycles are used in ethylene plants.

Refrigeration systems use power to compress the refrigerant. The power can be estimated using the cooling duty and the refrigerator coefficient of performance (*COP*).

$$COP = \frac{\text{Refrigeration produced (Btu/hr or MW)}}{\text{Shaft work used (Btu/hr or MW)}} \tag{3.2}$$

The *COP* is a strong function of the temperature range over which the refrigeration cycle operates. For an ideal refrigeration cycle (a reverse Carnot cycle), the *COP* is:

$$COP = \frac{T_e}{(T_c - T_e)} \tag{3.3}$$

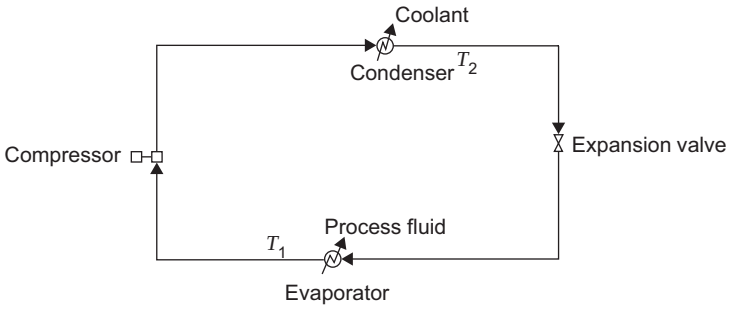


Fig. 3.5 Simple refrigeration cycle.

where: T_e = evaporator absolute temperature (K)
T_c = condenser absolute temperature (K)

The *COP* of real refrigeration cycles is always less than the Carnot efficiency. It is usually about 0.6 times the Carnot efficiency for a simple refrigeration cycle, but can be as high as 0.9 times the Carnot efficiency if complex cycles are used. If the temperature range is too large, then it may be more economical to use a cascaded refrigeration system, in which a low-temperature cycle rejects heat to a higher-temperature cycle that rejects heat to cooling water or ambient air. Good overviews of refrigeration cycle design are given by Dincer (2017), Stoecker (1998), and Hundy et al. (2008).

The operating cost of a refrigeration system can be determined from the power consumption and the price of power. Refrigeration systems are usually purchased as packaged modular plants, and the capital cost can be estimated using commercial cost estimating software, as described in Section 7.10. An approximate correlation for the capital cost of packaged refrigeration systems is also given in Table 7.2.

Example 3.3

Estimate the annual operating cost of providing refrigeration to a condenser with duty 1.2 MW operating at −5 °C. The refrigeration cycle rejects heat to cooling water that is available at 40 °C and has an efficiency of 80% of the Carnot cycle efficiency. The plant operates for 8000 hours per year, and electricity costs $0.06/kWh.

Solution

The refrigeration cycle needs to operate with an evaporator temperature below −5 °C, say at −10 °C or 263 K. The condenser must operate above 40 °C, say at 45 °C (318 K).

For this temperature range the Carnot cycle efficiency is:

$$COP = \frac{T_e}{(T_c - T_e)} = \frac{263}{318 - 263} = 4.78 \tag{3.3}$$

If the cycle is 80% efficient, then the actual $COP = 4.78 \times 0.8 = 3.83$

The shaft work needed to supply 1.2 MW of cooling is given by:

$$\text{Shaft work required} = \frac{\text{Cooling duty}}{COP} = \frac{1.2}{3.83} = 0.313 \text{ MW}$$

The annual operating cost is then = 313 kW × 8000 h/y × 0.06 $/kWh = 150,000 $/y

3.2.7 Water

The water required for general purposes on a site will usually be taken from the local mains supply, unless a cheaper source of suitable quality water is available from a river, lake, or well. Raw water is brought in to make up for losses in the steam and cooling water systems and is also treated to generate demineralized and deionized water for process use. Water is also used for process cleaning operations and to supply fire hydrants.

The price of water varies strongly by location, depending on fresh water availability. Water prices are often set by local government bodies and often include a charge for waste water rejection. This charge is usually applied on the basis of the water consumed by the plant, regardless of whether that water is actually rejected as a liquid (as opposed to being lost as vapor or incorporated into a product by reaction). A very rough estimate of water costs can be made by assuming $2 per 1000 gal ($0.5 per metric ton).

Demineralized water

Demineralized water, from which all the minerals have been removed by ion exchange, is used where pure water is needed for process use and as boiler feed-water. Mixed and multiple-bed ion exchange units are used, with one resin converting the cations to hydrogen and the other removing the anions. Water with less than 1 part per million of dissolved solids can be produced. The design of ion exchange units is discussed in Section 16.5.5. Demineralized water typically costs about double the price of raw water, but this obviously varies strongly with the mineral content of the water and the disposal cost of blowdown from the demineralization system. A correlation for the cost of a water ion exchange plant is given in Table 7.2.

3.2.8 Compressed air

Compressed air is needed for general use, oxidation reactions, air strippers, aerobic fermentation processes, and pneumatic control actuators that are used for plant control. Air is normally distributed at a mains pressure of 6 bar (100 psig), but large process air requirements are typically met with stand-alone air blowers or compressors. Rotary and reciprocating single-stage or two-stage compressors are used to supply utility and instrument air. Instrument air must be dry and clean (free from oil). Air is usually dried by passing it over a packed bed of molecular sieve adsorbent. For most applications, the adsorbent is periodically regenerated using a temperature swing cycle. Temperature swing adsorption (TSA) is discussed in more detail in Section 16.2.1.

Air at 1 atmosphere pressure is freely available in most chemical plants. Compressed air can be priced based on the power needed for compression (see Section 20.6). Drying the air—for example, for instrument air—typically adds about \$0.005 per standard m^3 (\$0.14/1000 scf).

Cooling air

Ambient air is used as a coolant in many process operations; for example, air-cooled heat exchangers, cooling towers, solids coolers, and prilling towers. If the air flow is caused by natural draft, then the cooling air is free, but the air velocity will generally be low, leading to high equipment cost. Fans or blowers are commonly used to ensure higher air velocities and reduce equipment costs. The cost of providing cooling air is then the cost of operating the fan, which can be determined from the fan power consumption. Cooling fans typically operate with very high flow rates and very low pressure drop, on the order of a few inches of water. The design of a cooling fan is illustrated in the discussion of air-cooled heat exchangers in Section 19.16.

3.2.9 Nitrogen

Where a large quantity of inert gas is required for the inert blanketing of tanks and for purging (see Chapter 10), this will usually be supplied from a central facility. Nitrogen is normally used and can be manufactured on site in an air liquefaction plant or purchased as a liquid in tankers.

Nitrogen and oxygen are usually purchased from one of the industrial gas companies via pipeline or a small dedicated "over-the-fence" plant. The price varies depending on local power costs, but is typically in the range of \$0.01 to \$0.03 per lb for large facilities.

3.3 Energy recovery

Process streams at HP or high temperature contain energy that can be usefully recovered. Whether it is economic to recover the energy content of a particular stream depends on the value of the energy that can be usefully extracted and the cost of recovery. The value of the energy is related to the marginal cost of energy at the site. The cost of recovery will be the capital and operating cost of any additional equipment required. If the savings exceed the total annualized cost, including capital charges, then the energy recovery will usually be worthwhile. Maintenance costs should be included in the annualized cost (see Chapter 9).

Some processes, such as air separation, depend on efficient energy recovery for economic operation, and in all processes the efficient use of energy will reduce product cost.

When setting up process simulation models, the design engineer needs to pay careful attention to operations that have an impact on the energy balance and heat use within the process. Some common problems to watch out for include:

1. Avoid mixing streams at very different temperatures. This usually represents a loss of heat (or cooling) that could be better used in the process.
2. Avoid mixing streams at different pressures. The mixed stream will be at the lowest pressure of the feed streams. The higher-pressure streams will undergo cooling as a result of adiabatic expansion. This may lead to increased heating or cooling requirements or lost potential to recover shaft work during the expansion.
3. Segment heat exchangers to avoid internal pinches. This is particularly necessary for exchangers where there is a phase change. When a liquid is heated, boiled, and superheated, the variation of stream temperature with enthalpy added looks like Fig. 3.6. Liquid is heated to the boiling point (A-B), then the heat of vaporization is added (B-C), and the vapor is superheated (C-D). This is a different temperature—enthalpy profile than a straight line between the initial and final states (A-D). If the stream in Fig. 3.6 were matched against a heat source that had

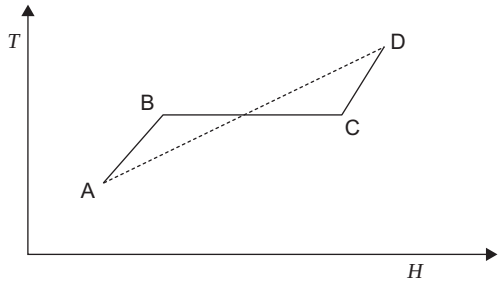


Fig. 3.6 Temperature–enthalpy profile for a stream that is vaporized and superheated.

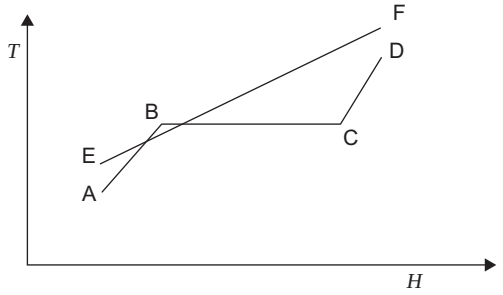


Fig. 3.7 Heat transfer to a stream that is vaporized and superheated.

a temperature profile like line E-F in Fig. 3.7, then the exchanger would appear feasible based on the inlet and outlet temperatures, but would in fact be infeasible because of the cross-over of the temperature profiles at B. A simple way to avoid this problem is to break up the preheat, boiling, and superheat into three exchangers in the simulation model, even if they will be carried out in a single piece of equipment in the final design. The same problem also occurs with condensers that incorporate desuperheat and subcooling.

4. Check for heat of mixing. This is important whenever acids or bases are mixed with water. If the heat of mixing is large, two or more stages of mixing with intercoolers may be needed. If a large heat of mixing is expected but is not predicted by the model, then check that the thermodynamic model includes heat of mixing effects.
5. Remember to allow for process inefficiency and design margins. For example, when sizing a fired heater, if process heating is carried out in the radiant section only, the heating duty calculated in the simulation is only 60% of the total furnace duty (see Sections 3.2.2 and 19.17). The operating duty will then be the process duty divided by 0.6. The design duty must be increased further by a suitable design factor, say 10%. The design duty of the fired heater is then $1.1/0.6 = 1.83$ times the process duty calculated in the simulation.

Some of the techniques used for energy recovery in chemical process plants are described briefly in the following sections. The references cited give fuller details of each technique. Miller (1968) gives a comprehensive review of process energy systems, including heat exchange and power recovery from HP fluid streams. Kenney (1984) reviews the application of thermodynamic principles to energy recovery in the process industries. Zhu (2014) and Knopf (2012) provide comprehensive treatments of energy recovery and process energy optimization. Kemp (2007) gives a detailed description of pinch analysis and several other methods for heat recovery.

3.3.1 Heat exchange

The most common energy-recovery technique is to use the heat in a high-temperature process stream to heat a colder stream. This saves part or all of the cost of heating the cold stream, as well as part or all of the cost of cooling the hot stream. Conventional shell and tube exchangers are normally used. The cost of the heat-exchange surface may be increased relative to using a hot utility as a heat source due to the reduced-temperature driving forces, or it may be decreased due to needing fewer exchangers. The cost of recovery will be reduced if the streams are located conveniently close within the plant.

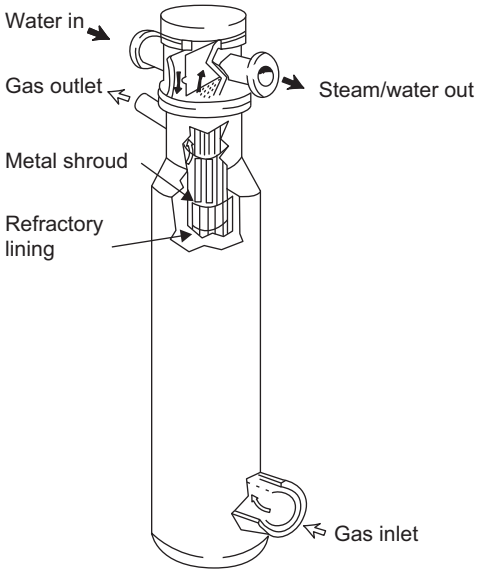


Fig. 3.8 Reformed gas waste–heat boiler arrangement of vertical U-tube water tube boiler. *Reprinted by permission of the Council of the Institution of Mechanical Engineers from the Proceedings of the Conference on Energy Recovery in the Process Industries, London, 1975.*

The amount of energy that can be recovered depends on the temperature, flow, heat capacity, and temperature change possible in each stream. A reasonable temperature-driving force must be maintained to keep the exchanger area to a practical size. The most efficient exchanger will be the one in which the shell and tube flows are truly counter-current. Multiple tube-pass exchangers are usually used for practical reasons. With multiple tube passes, the flow is part counter-current and part co-current, and temperature crosses can occur, which reduce the efficiency of heat recovery (see Chapter 19). In cryogenic processes, where heat recovery is critical to process efficiency, brazed or welded plate exchangers are used to obtain true counter-current performance, and very low-temperature approaches on the order of a few degrees Celsius are common.

The hot process streams leaving a reactor or a distillation column are frequently used to preheat the feed streams ("feed-effluent" or "feed-bottoms" exchangers).

In an industrial process there will be many hot and cold streams, and there will be an optimum arrangement of the streams for energy recovery by heat exchange. The problem of synthesizing a network of heat exchangers has been the subject of much research and is covered in more detail in Section 3.5.

3.3.2 Waste-heat boilers

If the process streams are at a sufficiently high temperature and there are no attractive options for process-to-process heat transfer, then the heat recovered can be used to generate steam.

Waste-heat boilers are often used to recover heat from furnace flue gases and to process gas streams from high-temperature reactors. The pressure and superheat temperature of the steam generated depend on the temperature of the hot stream and the approach temperature permissible at the boiler exit. As with any heat-transfer equipment, the area required increases as the mean temperature driving force (log mean ΔT) is reduced. The permissible exit temperature may also be limited by process considerations. If the gas stream contains water vapor and soluble corrosive gases, such as HCl or SO_2, the exit gas temperature must be kept above the dew point.

Hinchley (1975) discusses the design and operation of waste heat boilers for chemical plants. Both fire-tube and water-tube boilers are used. A typical arrangement of a water-tube boiler on a reformer furnace is shown in Fig. 3.8 and a fire-tube boiler in Fig. 3.9.

The application of a waste-heat boiler to recover energy from the reactor exit streams in a nitric acid plant is shown in Fig. 3.10. The selection and operation of waste heat boilers for industrial furnaces are discussed by Dryden (2013).

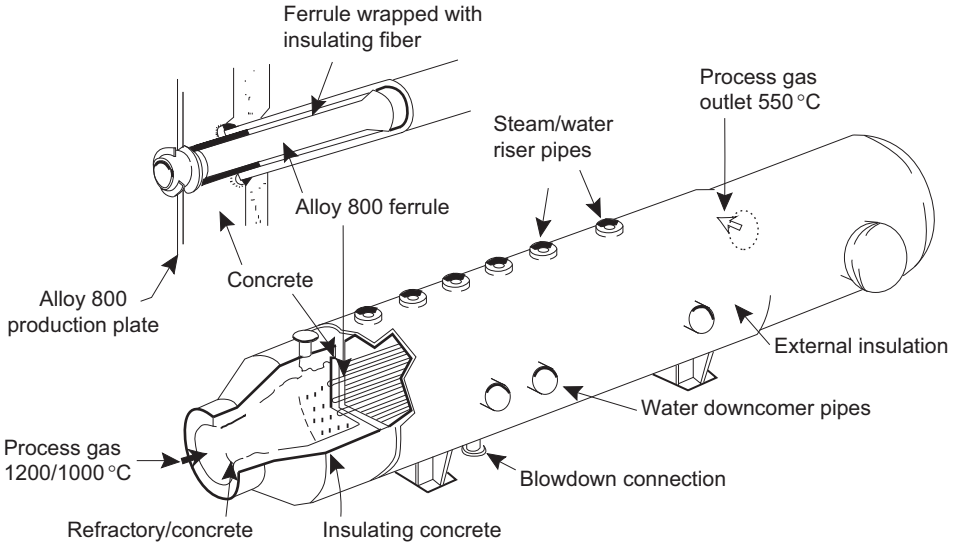
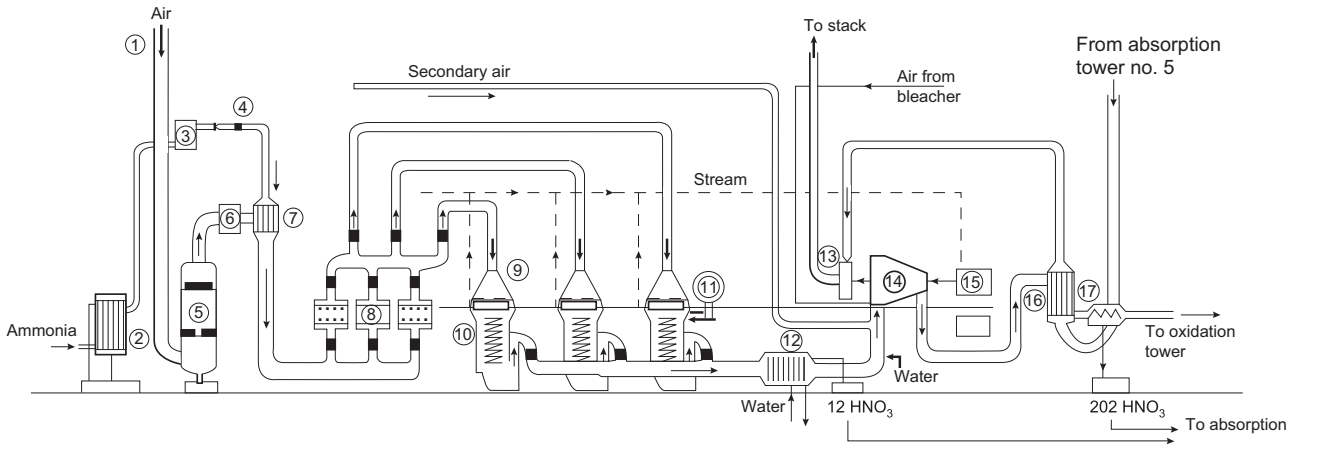


Fig. 3.9 Reformed gas waste-heat boiler, principal features of typical natural circulation fire-tube boilers. *Reprinted by permission of the Council of the Institution of Mechanical Engineers from the Proceedings of the Conference on Energy Recovery in the Process Industries, London, 1975.*



1. Air entry
2. Ammonia vaporiser
3. Ammonia filter
4. Control valves
5. Air-scrubbing tower
6. Air preheater
7. Gas mixer
8. Gas filters
9. Converters
10. Lamont boilers
11. Steam drum
12. Gas cooler No. 1
13. Exhaust turbine
14. Compressor
15. Steam turbine
16. Heat exchanger
17. Gas cooler No. 2

(From nitric acid manufacture, Miles (1961), with permission)

Fig. 3.10 Connections of a nitric acid plant, intermediate-pressure type.

3.3.3 High-temperature reactors

If a reaction is highly exothermic, cooling will be needed. If the reactor temperature is high enough, the heat removed can be used to generate steam. The lowest steam pressure normally used in the process industries is about 2.7 bar (25 psig), so any reactor with a temperature above 150 °C is a potential steam generator. Steam is preferentially generated at as high a pressure as possible, as HP steam is more valuable than LP steam (see Section 3.2.3). If the steam production exceeds the site steam requirements, some steam can be fed to condensing turbines to produce electricity to meet site power needs.

Three systems are used:

1. Fig. 3.11(*a*). An arrangement similar to a conventional water-tube boiler. Steam is generated in cooling pipes within the reactor and separated in a steam drum.
2. Fig. 3.11(*b*). Similar to the first arrangement but with the water kept at high pressure to prevent vaporization. The HP water is flashed to steam at a lower pressure in a flash drum. This system gives more responsive control over the reactor temperature.

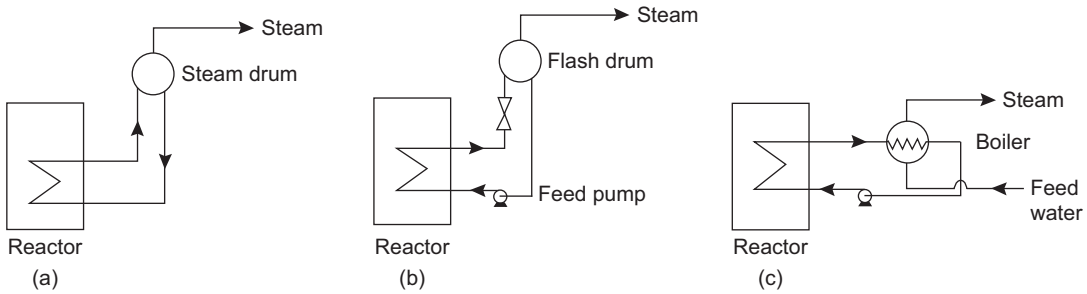


Fig. 3.11 Steam generation.

3. Fig. 3.11(*c*). In this system a heat-transfer fluid, such as Dowtherm A (see Section 3.2.4 and Singh [1985] for details of heat-transfer fluids) is used to avoid the need for HP tubes. The steam is raised in an external boiler.

3.3.4 High-pressure process streams

Where HP gas or liquid process streams are throttled to lower pressures, energy can be recovered by carrying out the expansion in a suitable turbine.

Gas streams

The economic operation of processes that involve the compression and expansion of large quantities of gases—such as ammonia synthesis, nitric acid production, and air separation—depends on the efficient recovery of the energy of compression. The energy recovered by expansion is often used to drive the compressors directly, as shown in Fig. 3.10. If the gas contains condensable components, it may be advisable to consider heating the gas by heat exchange with a higher-temperature process stream before expansion. The gas can then be expanded to a lower pressure without condensation and the power generated increased.

The process gases do not have to be at a particularly high pressure for expansion to be economical if the gas flow rate is high. For example, Luckenbach (1978) in U.S. patent 4,081,508 describes a process for recovering power from the off-gas from a fluid catalytic cracking process by expansion from about 2 to 3 bar (15 to 25 psig) down to just over atmospheric pressure (1.5 to 2 psig).

The energy recoverable from the expansion of a gas can be estimated by assuming polytropic expansion; see Section 20.6.3 and Example 20.4. The design of turboexpanders for the process industries is discussed by Bloch et al. (1982).

Liquid streams

As liquids are essentially incompressible, less energy is stored in a compressed liquid than a gas; however, it is often worth considering power recovery from HP liquid streams (>15 bar), as the equipment required is relatively simple and inexpensive. Centrifugal pumps are used as expanders and are often coupled directly to other pumps. The design, operation, and cost of energy recovery from HP liquid streams is discussed by Jenett (1968), Chada (1984), and Buse (1981).

3.3.5 Heat pumps

A heat pump is a device for raising low-grade heat to a temperature at which the heat can be used. It pumps the heat from a low-temperature source to the higher-temperature sink, using a small amount of energy relative to the heat energy recovered. A heat pump is essentially the same as a refrigeration cycle (Section 3.2.6 and Fig. 3.5), but the objective is to deliver heat to the process in the condensation step of the cycle, as well as (or instead of) removing heat in the evaporation step.

Heat pumps are increasingly finding applications in the process industries. A typical application is the use of the low-grade heat from the condenser of a distillation column to provide heat for the reboiler; see Barnwell and Morris (1982) and Meili (1990). Heat pumps are also used with dryers, with heat being abstracted from the exhaust air and used to preheat the incoming air.

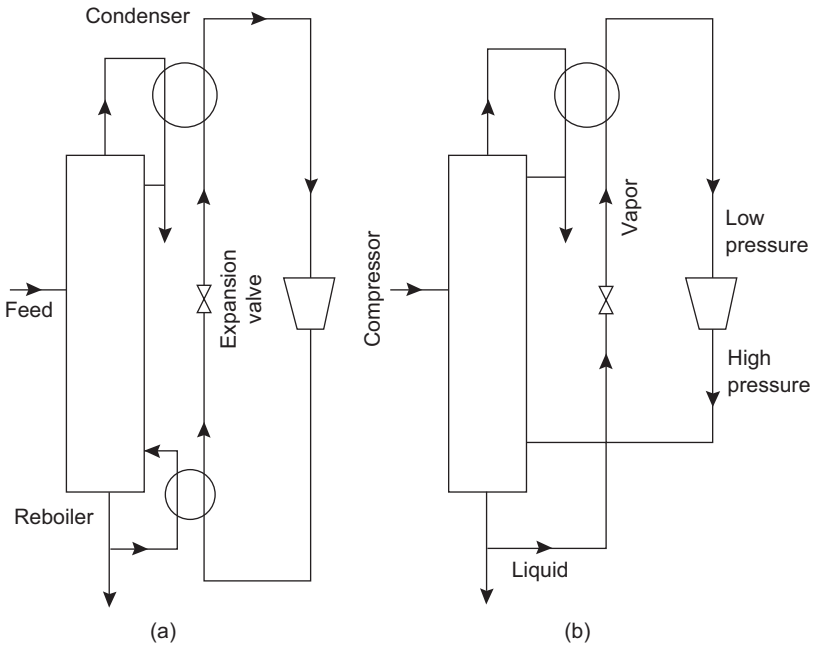


Fig. 3.12 Distillation column with heat pump. (*a*) Separate refrigerant circuit. (*b*) Using column fluid as the refrigerant.

Details of the thermodynamic cycles used for heat pumps can be found in most textbooks on engineering thermodynamics, and in Reay and MacMichael (1988). In the process industries, heat pumps operating on the mechanical vapor compression cycle are normally used. A vapor compression heat pump applied to a distillation column is shown in Fig. 3.12(*a*). The working fluid, usually a commercial refrigerant, is fed to the reboiler as a vapor at HP and condenses, giving up heat to vaporize the process fluid. The liquid refrigerant from the reboiler is then expanded over a throttle valve, and the resulting wet vapor is fed to the column condenser. In the condenser the wet refrigerant is dried, taking heat from the condensing process vapor. The refrigerant vapor is then compressed and recycled to the reboiler, completing the working cycle.

If the conditions are suitable, the process fluid can be used as the working fluid for the heat pump. This arrangement is shown in Fig. 3.12(*b*). The hot process liquid at HP is expanded over the throttle valve and fed to the condenser to provide cooling to condense the vapor from the column. The vapor from the condenser is compressed and returned to the base of the column. In an alternative arrangement, the process vapor is taken from the top of the column, compressed, and fed to the reboiler to provide heating.

The "efficiency" of a heat pump is measured by the heat pump coefficient of performance, COP_h:

$$COP_h = \frac{\text{energy delivered at higher temperature}}{\text{energy input to the compressor}} \tag{3.4}$$

The COP_h depends principally on the working temperatures. Heat pumps are more efficient (higher COP_h) when operated over a narrow temperature range. They are thus most often encountered on distillation columns that separate close-boiling compounds. Note that the COP_h of a heat pump is not the same as the COP of a refrigeration cycle (Section 3.2.6).

The economics of the application of heat pumps in the process industries is discussed by Holland and Devotta (1986). Details of the application of heat pumps in a wide range of industries are given by Moser and Schnitzer (1985).

3.4 Waste stream combustion

Process waste products that contain significant quantities of combustible material can be used as low-grade fuels for raising steam or direct process heating. Their use will only be economic if the intrinsic value of the fuel justifies

the cost of special burners and other equipment needed to burn the waste. If the combustible content of the waste is too low to support combustion, the waste must be supplemented with higher-calorific-value primary fuels.

3.4.1 Reactor off-gases

Reactor off-gases (vent gas) and recycle stream purges are often of high enough calorific value to be used as fuels. Vent gases will typically be saturated with organic compounds such as solvents and high-volatility feed compounds. The calorific value of a gas can be calculated from the heats of combustion of its constituents; the method is illustrated in Example 3.4.

Other factors that, together with the calorific value, determine the economic value of an off-gas as a fuel are the quantity available and the continuity of supply. Waste gases are best used for steam raising rather than for direct process heating, as this decouples the source from the use and gives greater flexibility.

Example 3.4 Calculation of waste-gas calorific value

The typical vent gas analysis from the recycle stream in an oxyhydrochlorination process for the production of dichloroethane (DCE) (British patent BP 1,524,449) is given here, with percentages on volume basis.

$$O_2\ 7.96,\ CO_2 + N_2\ 87.6,\ CO\ 1.79, C_2H_4\ 1.99, C_2H_6\ 0.1,\ DCE\ 0.54$$

Estimate the vent gas calorific value.

Solution

Component calorific values, from Perry and Chilton (1973)

$$CO\ 67.6\ \text{kcal/mol} = 283\ \text{kJ/mol}$$

$$C_2H_4\ 372.8 = 1560.9$$

$$C_2H_6\ 337.2 = 1411.9$$

The value for DCE can be estimated from the heats of formation.

Combustion reaction:

$$C_2H_4Cl_2(g) + 2\frac{1}{2}O_2(g) \rightarrow 2CO_2(g) + H_2O(g) + 2HCl(g)$$

The heats of formation ΔH_f° are given in Appendix C, which is available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

$$CO_2 = -393.8\ \text{kJ/mol}$$

$$H_2O = -242.0$$

$$HCl = -92.4$$

$$DCE = -130.0$$

$$\Delta H_c^\circ = \sum \Delta H_f^\circ\ \text{products} - \sum \Delta H_f^\circ\ \text{reactants}$$

$$= [2(-393.8) - 242.0 + 2(-92.4)] - [-130.0]$$

$$= -1084.4\ \text{kJ}$$

Estimation of vent gas calorific value, basis 100 mol.

Component	mol/100 mol		Calorific Value		Heating Value (kJ/mol)
CO	1.79	×	283.0	=	506.6
C_2H_4	1.99		1560.9		3106.2
C_2H_6	0.1		1411.9		141.2
DCE	0.54		1084.4		585.7
				Total	4339.7

$$\text{Calorific value of vent gas} = \frac{4339.7}{100} = 43.4 \text{ kJ/mol}$$

$$= \frac{43.4}{22.4} \times 10^3 = 1938 \text{ kJ/m}^3 (52 \text{ Btu/ft}^3) \text{ at 1 bar, 0 °C}$$

This calorific value is very low compared with 37 MJ/m^3 (1000 Btu/ft^3) for natural gas. The vent gas is barely worth recovery, but if the gas has to be burnt to avoid pollution, it could be used in an incinerator such as that shown in Fig. 3.13, giving a useful steam production to offset the cost of disposal.

3.4.2 Liquid and solid wastes

Combustible liquid and solid waste can be disposed of by burning, which is usually preferred to dumping. Incorporating a steam boiler in the incinerator design will enable an otherwise unproductive, but necessary, operation to save energy. If the combustion products are corrosive, corrosion-resistant materials will be needed, and the flue gases must be scrubbed to reduce air pollution. An incinerator designed to handle chlorinated and other liquid and solid wastes is shown in Fig. 3.13. This incinerator incorporates a steam boiler and a flue-gas scrubber. The disposal of chlorinated wastes is discussed by Santoleri (1973).

Dunn and Tomkins (1975) discuss the design and operation of incinerators for process wastes. They give particular attention to the need to comply with the current clean air legislation and the problem of corrosion and erosion of refractories and heat-exchange surfaces.

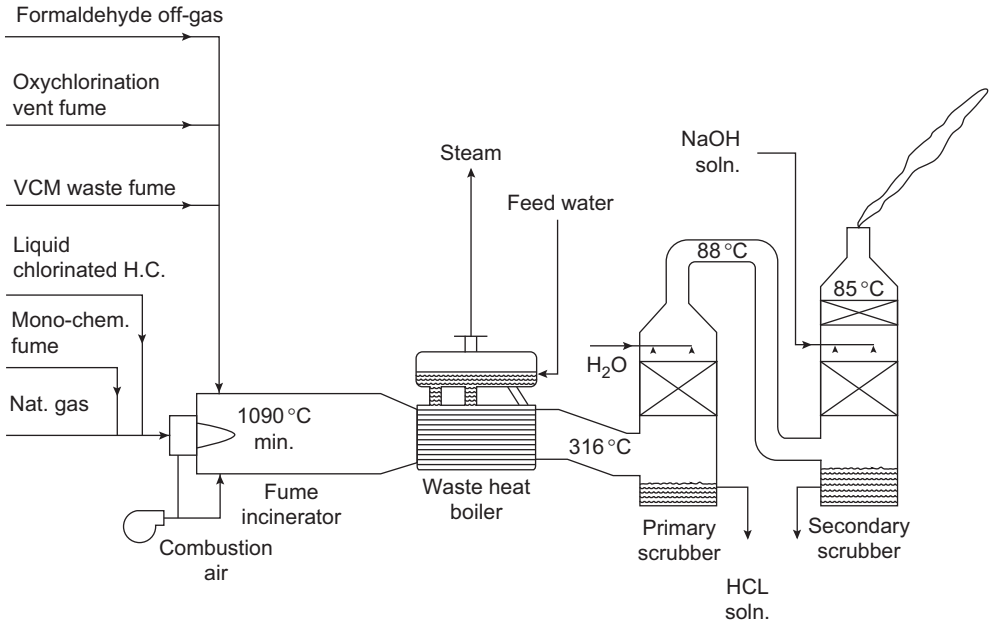


Fig. 3.13 Typical incinerator–heat recovery–scrubber system for vinyl chloride–monomer process waste. *Courtesy John Thurley Ltd.*

3.5 Heat exchanger networks

The design of a heat exchanger network for a simple process with only one or two streams that need heating and cooling is usually straightforward. When there are multiple hot and cold streams, the design is more complex, and there may be many possible heat-exchange networks. The design engineer must determine the optimum extent of heat recovery while ensuring that the design is flexible to changes in process conditions and can be started up and operated easily and safely.

In the 1980s, there was a great deal of research into design methods for heat exchanger networks; see Gundersen and Naess (1988). One of the most widely applied methods that emerged was a set of techniques termed *pinch technology* that was developed by Bodo Linnhoff and his collaborators at ICI, Union Carbide, and the University of Manchester. The term derives from the fact that in a plot of the system temperatures versus the heat transferred, a *pinch* usually occurs between the hot stream and cold stream curves (see Fig. 3.19). It has been shown that the pinch represents a distinct thermodynamic break in the system and that for minimum energy requirements, heat should not be transferred across the pinch (Linnhoff et al. [1982]).

In this section the fundamental principles of the pinch technology method for energy integration will be outlined and illustrated with reference to a simple problem. The method and its applications are described fully in a guide published by the Institution of Chemical Engineers, Kemp (2007); see also Douglas (1988), Knopf (2012), Smith (2016), Zhu (2014), and El-Halwagi (2006).

3.5.1 Pinch technology

The development and application of the method can be illustrated by considering the problem of recovering heat between four process streams: two hot streams that require cooling and two cold streams that must be heated. The process data for the streams are set out in Table 3.1. Each stream starts from a source temperature T_s and is to be heated or cooled to a target temperature T_t. The heat capacity flow rate of each stream is shown as CP. For streams where the specific heat capacity can be taken as a constant and there is no phase change, CP will be given by:

$$CP = mC_p \tag{3.5}$$

where m = mass flow rate, kg/s

C_p = average specific heat capacity between T_s and T_t kJ kg^{-1}°C^{-1}

The heat load shown in the table is the total heat required to heat or cool the stream from the source to the target temperature.

There is clearly scope for energy integration between these four streams. Two require heating and two cooling, and the stream temperatures are such that heat can be transferred from the hot to the cold streams. The task is to find the best arrangement of heat exchangers to achieve the target temperatures.

Simple two-stream problem

Before investigating the energy integration of the four streams shown in Table 3.1, the use of a temperature–enthalpy diagram will be illustrated for a simple problem involving only two streams. The general problem of heating and cooling two streams from source to target temperatures is shown in Fig. 3.14. Some heat is exchanged between the streams in the heat exchanger. Additional heat to raise the cold stream to the target temperature is provided by the hot utility (usually steam) in the heater, and additional cooling to bring the hot stream to its target temperature is provided by the cold utility (usually cooling water) in the cooler.

TABLE 3.1 Data for heat integration problem

Stream number	Type	Heat capacity flow rate *CP*, kW/°C	*Ts*°C	*Tt*°C	Heat load kW
1	Hot	3.0	180	60	360
2	Hot	1.0	150	30	120
3	Cold	2.0	20	135	230
4	Cold	4.5	80	140	270

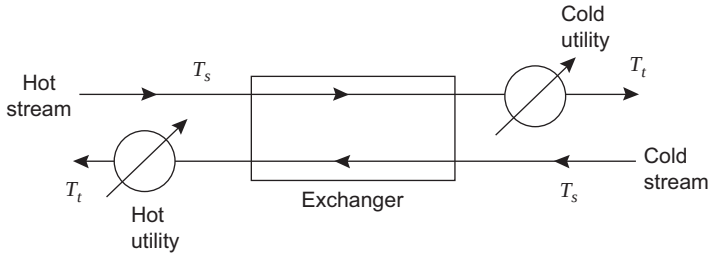


Fig. 3.14 Two-stream exchanger problem.

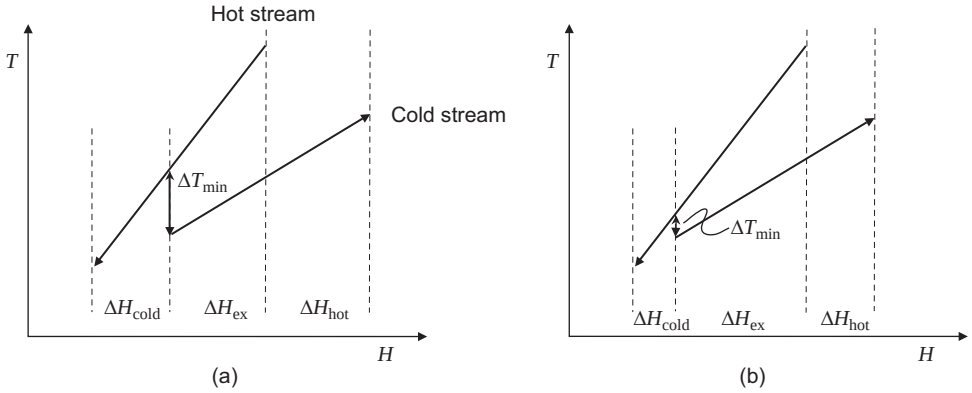


Fig. 3.15 Temperature–enthalpy (*T-H*) diagram for two-stream example.

In Fig. 3.15(*a*) the stream temperatures are plotted on the y-axis and the enthalpy change of each stream on the x-axis. This is known as a *temperature–enthalpy (T-H) diagram*. For heat to be exchanged, a minimum temperature difference must be maintained between the two streams. This is shown as ΔT_{min} on the diagram. The practical minimum temperature difference in a heat exchanger will usually be between 5° and 30 °C; see Chapter 19.

The slope of the lines in the *T-H* plot is proportional to $1/CP$, because $\Delta H = CP \times \Delta T$, so $dT/dH = 1/CP$. Streams with low heat capacity flow rate thus have steep slopes in the *T-H* plot, and streams with high heat capacity flow rate have shallow slopes.

The heat transferred between the streams is given by the range of enthalpy over which the two curves overlap each other and is shown on the diagram as ΔH_{ex}. The heat transferred from the hot utility, ΔH_{hot}, is given by the part of the cold stream that is not overlapped by the hot stream. The heat transferred to the cold utility, ΔH_{cold}, is similarly given by the part of the hot stream that is not overlapped by the cold stream. The heats can also be calculated as:

$$\Delta H = CP \times (\textit{temperature change})$$

Because we are only concerned with changes in enthalpy, we can treat the enthalpy axis as a relative scale and slide either the hot stream or the cold stream horizontally. As we do so, we change the minimum temperature difference between the streams, ΔT_{min}, and also the amount of heat exchanged and the amounts of hot and cold utilities required.

Fig. 3.15(*b*) shows the same streams plotted with a lower value of ΔT_{min}. The amount of heat exchanged is increased, and the utility requirements have been reduced. The temperature-driving force for heat transfer has also been reduced, so the heat exchanger has both a larger duty and a smaller log-mean temperature difference. This leads to an increase in the heat transfer area required and in the capital cost of the exchanger. The capital cost increase is partially offset by capital cost savings in the heater and cooler, which both become smaller, as well as by savings in the costs of hot and cold utility. In general, there will be an optimum value of ΔT_{min}, as illustrated in Fig. 3.16. This optimum is usually rather flat over the range of 10° to 30 °C.

The maximum feasible heat recovery is reached at the point where the hot and cold curves touch each other on the *T-H* plot, as illustrated in Fig. 3.17. At this point, the temperature-driving force at one end of the heat exchanger is

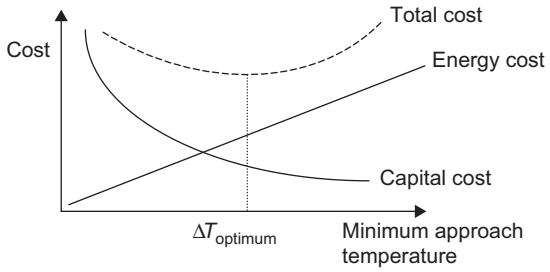


Fig. 3.16 The capital–energy trade-off in process heat recovery.

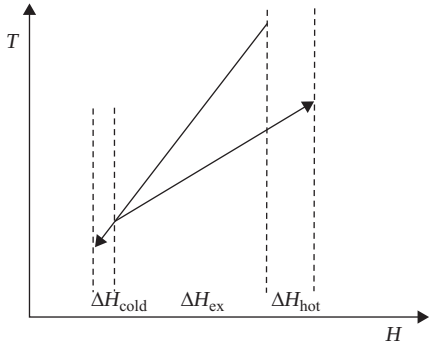


Fig. 3.17 Maximum feasible heat recovery for two-stream example.

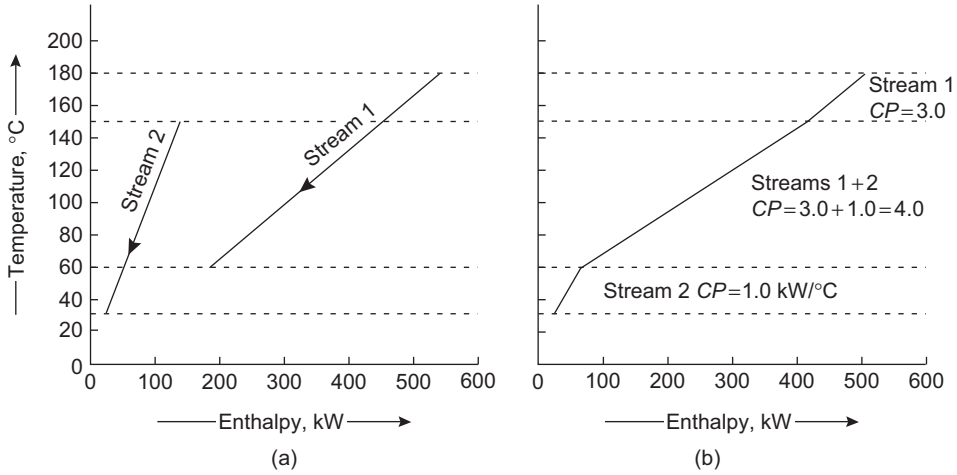


Fig. 3.18 Hot stream temperature vs. enthalpy. (*a*) Separate hot streams. (*b*) Composite hot streams. *CP*, * .

zero, and an infinite heat exchange surface is required, so the design is not practical. The exchanger is said to be *pinched* at the end where the hot and cold curves meet. In Fig. 3.17, the heat exchanger is pinched at the cold end.

It is not possible for the hot and cold streams to cross each other, as this would be a violation of the second law of thermodynamics and would give an infeasible design.

Four-stream problem

In Fig. 3.18(*a*) the hot streams given in Table 3.1 are shown plotted on a *T-E* diagram.

As the diagram shows changes in the enthalpy of the streams, it does not matter where a particular curve is plotted on the enthalpy axis as long as the curve runs between the correct temperatures. This means that where more than one stream appears in a temperature interval, the stream heat capacities can be added to form a composite curve, as shown in Fig. 3.18(*b*).

In Fig. 3.19, the composite curve for the hot streams and the composite curve for the cold streams are drawn with a minimum temperature difference—the displacement between the curves—of 10 °C. This implies that in any of the exchangers to be used in the network, the temperature difference between the streams will not be less than 10 °C.

As for the two-stream problem, the overlap of the composite curves gives a target for heat recovery, and the displacements of the curves at the top and bottom of the diagram give the hot and cold utility requirements. These will be the minimum values needed to satisfy the target temperatures. This is valuable information. It gives the designer target values for the utilities to aim for when designing the exchanger network. Any design can be compared with the minimum utility requirements to check if further improvement is possible.

In most exchanger networks the minimum temperature difference will occur at only one point. This is termed the *pinch*. In the problem being considered, the pinch occurs at between 90 °C on the hot stream curve and 80 °C on the cold stream curve.

For multistream problems, the pinch will usually occur somewhere in the middle of the composite curves, as illustrated in Fig. 3.19. The case when the pinch occurs at the end of one of the composite curves is termed a *threshold problem* and is discussed in Section 3.5.5.

Thermodynamic significance of the pinch

The pinch divides the system into two distinct thermodynamic regions. The region above the pinch can be considered a heat sink, with heat flowing into it, from the hot utility but no heat flow out of it. Below the pinch the converse is true. Heat flows out of the region to the cold utility. No heat flows across the pinch, as shown in Fig. 3.20(*a*).

If a network is designed in which heat is transferred from any hot stream at a temperature above the pinch (including hot utilities) to any cold stream at a temperature below the pinch (including cold utilities), then heat is transferred across the pinch. If the amount of heat transferred across the pinch is ΔH_{xp}, then to maintain energy balance, the hot utility and cold utility must both be increased by ΔH_{xp}, as shown in Fig. 3.20(*b*). Cross-pinch heat transfer thus always leads to consumption of both hot and cold utilities that is greater than the minimum values that could be achieved.

The pinch decomposition is useful in heat exchanger network design, as it decomposes the problem into two smaller problems. It also indicates the region where heat transfer matches are most constrained, at or near the pinch. When multiple hot or cold utilities are used, there may be other pinches, termed *utility pinches*, that cause further problem decomposition. Problem decomposition can be exploited in algorithms for automatic heat exchanger network synthesis.

3.5.2 The problem table method

The problem table is a numerical method for determining the pinch temperatures and the minimum utility requirements, introduced by Linnhoff and Flower (1978). It eliminates the sketching of composite curves, which

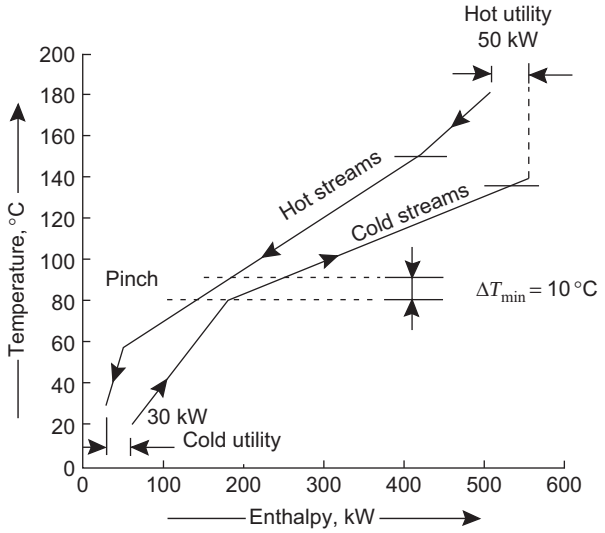


Fig. 3.19 Hot and cold stream composite curves.

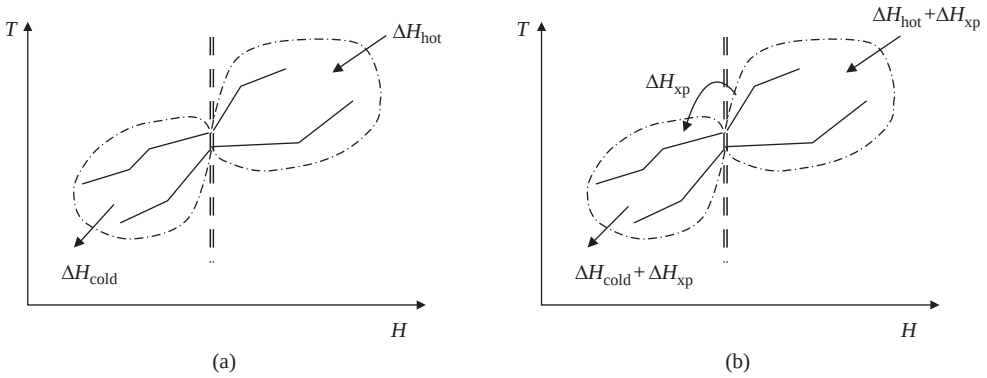


Fig. 3.20 Pinch decomposition.

can be useful if the problem is being solved manually. It is not widely used in industrial practice any more due to the wide availability of computer tools for pinch analysis (see Section 3.5.7).

The procedure is as follows:

1. Convert the actual stream temperatures T_{act} into interval temperatures T_{int} by subtracting half the minimum temperature difference from the hot stream temperatures and by adding half to the cold stream temperatures:

$$\text{hot streams } T_{int} = T_{act} - \frac{\Delta T_{min}}{2}$$

$$\text{cold streams } T_{int} = T_{act} + \frac{\Delta T_{min}}{2}$$

The use of the interval temperature rather than the actual temperatures allows the minimum temperature difference to be taken into account. $\Delta T_{min} = 10$ °C for the problem being considered (Table 3.2).

2. Note any duplicated interval temperatures. These are bracketed in Table 3.2.
3. Rank the interval temperatures in order of magnitude, showing the duplicated temperatures only once in the order (Table 3.3).

TABLE 3.2 Interval temperatures for $\Delta T_{min} = 10$ °C

Stream	Actual	Temperature	Interval	Temperature
1	180	60	175	55
2	150	30	145	25
3	20	135	(25)	140
4	80	140	85	(145)

TABLE 3.3 Ranked order of interval temperatures

Rank	Interval ΔT_n°C	Streams in interval
175 °C		
145	30	−1
140	5	4 − (2 + 1)
85	55	(3 + 4) − (1 + 2)
55	30	3 − (1 + 2)
25	30	3 − 2

Note: Duplicated temperatures are omitted. The interval ΔT and streams in the intervals are included, as they are needed for Table 3.4.

TABLE 3.4 Problem table

Interval	Interval temp. °C	ΔT_n-C	$\Sigma CP_c - \Sigma CP_h$* kW/°C	ΔH kW	Surplus or deficit
	175				
1	145	30	−3.0	−90	s
2	140	5	0.5	2.5	d
3	85	55	2.5	137.5	d
4	55	30	−2.0	−60	s
5	25	30	1.0	30	d

Note: The streams in each interval are given in Table 3.3.

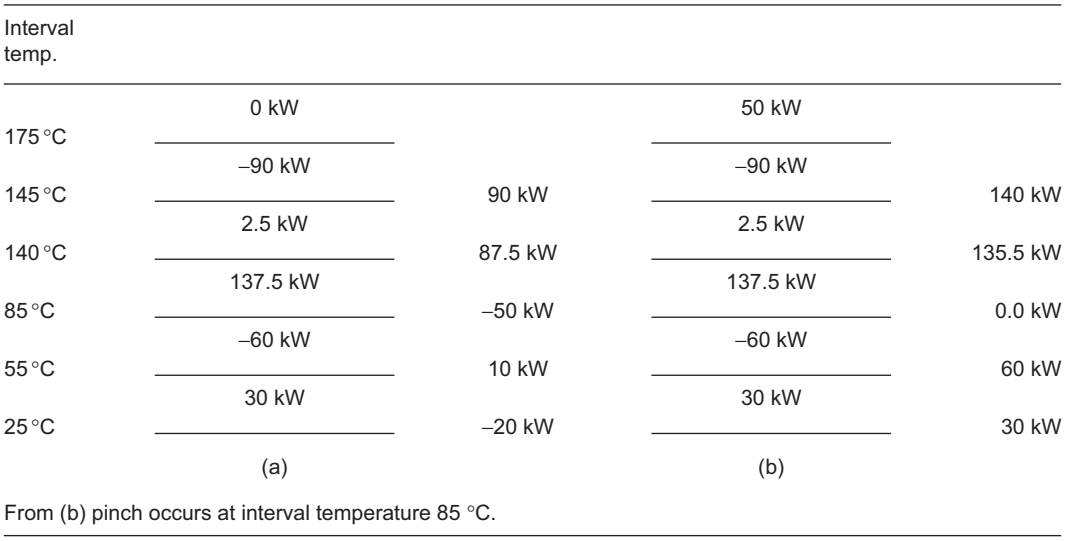


Fig. 3.21 Heat cascade.

4. Carry out a heat balance for the streams falling within each temperature interval:
For the nth interval:

$$\Delta H_n = (\Sigma CP_c - \Sigma CP_h)(\Delta T_n)$$

where ΔH_n = net heat required in the nth interval
ΣCP_c = sum of the heat capacities of all the cold streams in the interval
ΣCP_h = sum of the heat capacities of all the hot streams in the interval
ΔT_n = interval temperature difference = $(T_{n-1} - T_n)$

See Table 3.4.

5. "Cascade" the heat surplus from one interval to the next down the column of interval temperatures, as shown in Fig. 3.21(*a*).
Cascading the heat from one interval to the next implies that the temperature difference is such that the heat can be transferred between the hot and cold streams. The presence of a negative value in the column indicates that the temperature gradient is in the wrong direction and that the exchange is not thermodynamically possible.
This difficulty can be overcome if heat is introduced into the top of the cascade:

6. Introduce just enough heat to the top of the cascade to eliminate all the negative values; see Fig. 3.21(*b*).
Comparing the composite curve (see Fig. 3.19) with Fig. 3.21(*b*) shows that the heat introduced to the cascade is the minimum hot utility requirement and the heat removed at the bottom is the minimum cold utility required. The pinch occurs in Fig. 3.21(*b*) where the heat flow in the cascade is zero. This is as would be expected from the rule that for minimum utility requirements no heat flows across the pinch. In Fig. 3.21(*b*) the pinch is at an interval

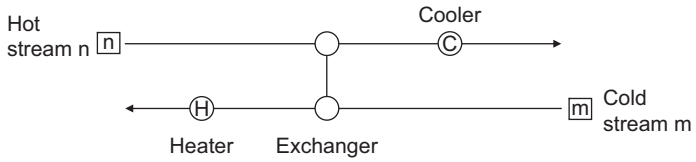


Fig. 3.22 Grid representation.

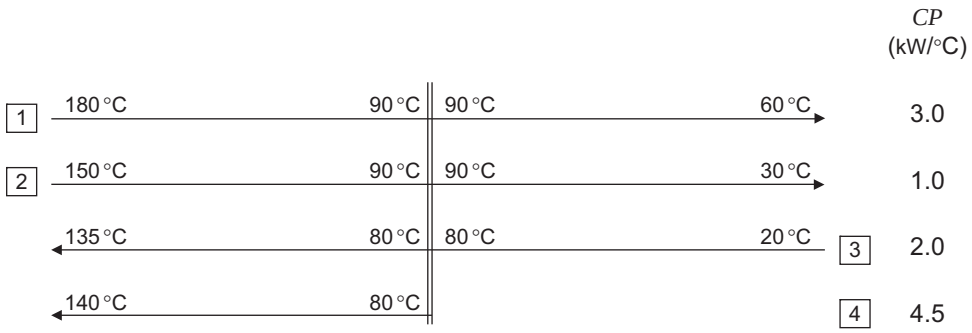


Fig. 3.23 Grid for four-stream problem.

temperature of 85 °C, corresponding to a cold stream temperature of 80 °C and a hot stream temperature of 90 °C, as was found using the composite curves.

It is not necessary to draw up a separate cascade diagram. This was done in Fig. 3.21 to illustrate the principle. The cascaded values can be added to the problem table as two additional columns; see Example 3.5.

Summary

For maximum heat recovery and minimum use of utilities:

1. Do not transfer heat across the pinch.
2. Do not use hot utilities below the pinch.
3. Do not use cold utilities above the pinch.

3.5.3 Heat exchanger network design

Grid representation

It is convenient to represent a heat exchanger network as a grid (Fig. 3.22). The process streams are drawn as horizontal lines, with the stream numbers shown in square boxes. Hot streams are drawn at the top of the grid and flow from left to right. The cold streams are drawn at the bottom and flow from right to left. The stream heat capacities *CP* are shown in a column at the end of the stream lines.

Heat exchangers are drawn as two circles connected by a vertical line. The circles connect the two streams between which heat is being exchanged; that is, the streams that would flow through the actual exchanger. Heaters and coolers can be drawn as a single circle, connected to the appropriate utility. If multiple utilities are used, then these can also be shown as streams. Exchanger duties are usually marked under the exchanger, and temperatures are also sometimes indicated on the grid diagram.

Network design for maximum energy recovery

The analysis carried out in Fig. 3.19 and Fig. 3.21 has shown that the minimum utility requirements for the problem set out in Table 3.1 are 50 kW of the hot and 30 kW of the cold utility and that the pinch occurs where the cold streams are at 80 °C and the hot streams are at 90 °C.

The grid representation of the streams is shown in Fig. 3.23. The vertical dotted lines represent the pinch and separate the grid into the regions above and below the pinch. Note that the hot and cold streams are off-set at the pinch because of the difference in pinch temperature.

For maximum energy recovery (minimum utility consumption) the best performance is obtained if no cooling is used above the pinch. This means that the hot streams above the pinch should be brought to the pinch temperature solely by exchange with the cold streams. The network design is therefore started at the pinch, finding feasible matches between streams to fulfill this aim. In making a match adjacent to the pinch the heat capacity CP of the hot stream must be equal to or less than that of the cold stream. This is to ensure that the minimum temperature difference between the curves is maintained. The slope of a line on the T-E diagram is equal to the reciprocal of the heat capacity. So, above the pinch the lines will converge if CP_h exceeds CP_c, and as the streams start with a separation at the pinch equal to ΔT_{min}, the minimum temperature condition would be violated. Every hot stream must be matched with a cold stream immediately above the pinch; otherwise, it will not be able to reach the pinch temperature.

Below the pinch the procedure is the same, with the aim being to bring the cold streams to the pinch temperature by exchange with the hot streams. For streams adjacent to the pinch, the criterion for matching streams is that the heat capacity of the cold stream must be equal to or greater than the hot stream to avoid breaking the minimum temperature difference condition. Every cold stream must be matched with a hot stream immediately below the pinch.

Network design above the pinch

$$CP_h \leq CP_c$$

1. Applying this condition at the pinch, stream 1 can be matched with stream 4 but not with stream 3.

Matching streams 1 and 4 and transferring the full amount of heat required to bring stream 1 to the pinch temperature gives:

$$\Delta H_{ex} = CP(T_s - T_{pinch})$$

$$\Delta H_{ex} = 3.0(180 - 90) = 270 \text{ kW}$$

This will also satisfy the heat load required to bring stream 4 to its target temperature:

$$\Delta H_{ex} = 4.5(140 - 80) = 270 \text{ kW}$$

2. Stream 2 can be matched with stream 3 while satisfying the heat capacity restriction. Transferring the full amount to bring stream 2 to the pinch temperature:

$$\Delta H_{ex} = 1.0(150 - 90) = 60 \text{ kW}$$

3. The heat required to bring stream 3 to its target temperature from the pinch temperature is:

$$\Delta H = 2.0(135 - 80) = 110 \text{ kW}$$

So a heater will have to be included to provide the remaining heat load:

$$\Delta H_{hot} = 110 - 60 = 50 \text{ kW}$$

This checks with the value given by the problem table in Fig. 3.21(*b*).

The proposed network design above the pinch is shown in Fig. 3.24.

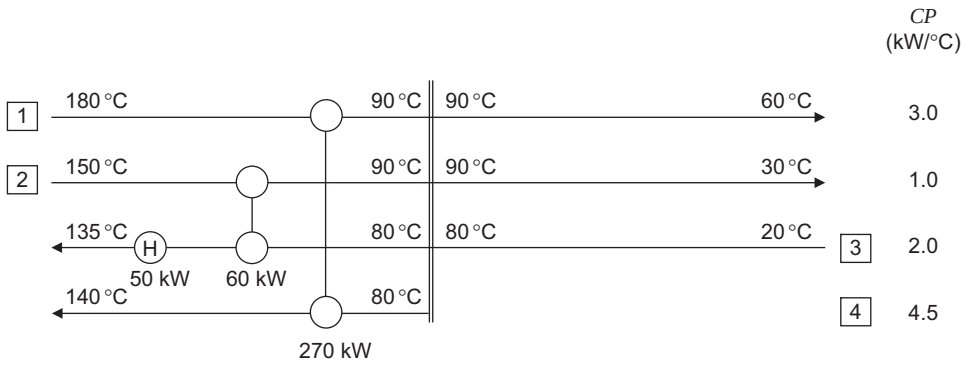


Fig. 3.24 Network design above the pinch.

Network design below the pinch

$$CP_h \geq CP_c$$

4. Stream 4 begins at the pinch temperature, $T_s = 80\ ^\circ C$ and so is not available for any matches below the pinch.
5. A match between stream 1 and 3 adjacent to the pinch will satisfy the heat capacity restriction but not one between streams 2 and 3. So stream 1 is matched with stream 3, transferring the full amount to bring stream 1 to its target temperature:

$$\Delta H_{ex} = 3.0(90 - 60) = 90\ \text{kW}$$

6. Stream 3 requires more heat to bring it to the pinch temperature; the amount needed:

$$\Delta H = 2.0(80 - 20) - 90 = 30\ \text{kW}$$

This can be provided from stream 2, as the match is now away from the pinch.
The rise in temperature of stream 3 will be given by:

$$\Delta T = \Delta H / CP$$

So transferring 30 kW will raise the temperature from the source temperature to:

$$20 + 30/2.0 = 35\ ^\circ C$$

and this gives a stream temperature difference on the outlet side of the exchanger of:

$$90 - 35 = 55\ ^\circ C$$

So the minimum temperature difference condition, 10 °C, will not be violated by this match.

7. Stream 2 needs further cooling to bring it to its target temperature, so a cooler must be included; the cooling required is:

$$\Delta H_{cold} = 1.0(90 - 30) - 30 = 30\ \text{kW}$$

which is the amount of the cold utility predicted by the problem table.
The proposed network for maximum energy recovery is shown in Fig. 3.25.

Stream splitting

If the heat capacities of streams are such that it is not possible to make a match at the pinch without violating the minimum temperature difference condition, then the heat capacity can be altered by splitting a stream. Dividing the stream will reduce the mass flow rates in each leg and hence the heat capacities. This is illustrated in Example 3.5.

Similarly, if there are not enough streams available to make all of the required matches at the pinch, then streams with large *CP* can be split to increase the number of streams.

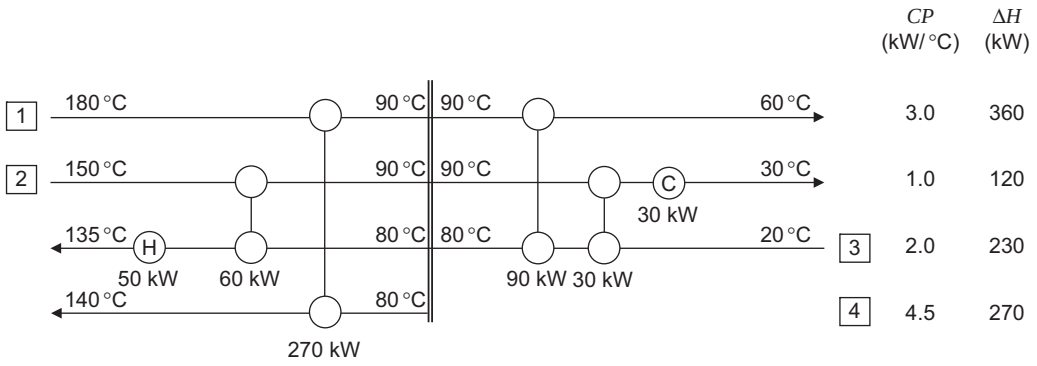


Fig. 3.25 Proposed heat exchanger network for $\Delta T_{min} = 10\ ^\circ C$.

Guide rules for stream matching and splitting are given in the *Institution of Chemical Engineers Guide*, Kemp (2007), and Smith (2016).

Summary

The guide rules for devising a network for maximum heat recovery are as follows:

1. Divide the problem at the pinch.
2. Design away from the pinch.
3. Above the pinch, match streams adjacent to the pinch, meeting the restriction:

$$CP_h \leq CP_c$$

4. Below the pinch, match streams adjacent to the pinch, meeting the restriction:

$$CP_h \geq CP_c$$

5. If the stream matching criteria cannot be satisfied, split a stream.
6. Maximize the exchanger heat loads.
7. Supply external heating only above the pinch and external cooling only below the pinch.

3.5.4 Minimum number of exchangers

The network shown in Fig. 3.25 was designed to give the maximum heat recovery and will therefore give the minimum consumption, and cost, of the hot and cold utilities.

This will not necessarily be the optimum design for the network. The optimum design will be that which gives the lowest total annualized cost, taking into account the capital cost of the system, in addition to the utility and other operating costs. The number of exchangers in the network, and their size, will determine the capital cost.

In Fig. 3.25 it is clear that there is scope for reducing the number of exchangers. The 30 kW exchanger between streams 2 and 3 can be deleted and the heat loads of the cooler and heater increased to bring streams 2 and 3 to their target temperatures. Heat would cross the pinch, and the consumption of the utilities would be increased. Whether the revised network would be better, or more economic, depends on the relative cost of capital and utilities and the operability of each design. For any network, there will be an optimum design that gives the least annual cost: capital charges plus utility and other operating costs. The estimation of capital and operating costs is covered in Chapters 7 and 8.

To find the optimum design, it is necessary to cost a number of alternative designs, seeking a compromise between the capital costs, determined by the number and size of the exchangers, and the utility costs, determined by the heat recovery achieved.

For simple networks, Holmann (1971) has shown that the minimum number of exchangers is given by:

$$Z_{min} = N' - 1 \tag{3.6}$$

where Z_{min} = minimum number of exchangers needed, including heaters and coolers
N' = the number of streams, including the utilities

For complex networks, a more general expression is needed to determine the minimum number of exchangers:

$$Z_{min} = N' + L' - S \tag{3.7}$$

where L' = the number of internal loops present in the network
S = the number of independent branches (subsets) that exist in the network

A loop exists where a closed path can be traced through the network. A loop in the network shown in Fig. 3.25 is shown in Fig. 3.26. The presence of a loop indicates that there is scope for reducing the number of exchangers.

For a full discussion of Equation 3.7 and its applications see Linnhoff et al. (1979), Smith (2016), Zhu (2014), or Kemp (2007).

In summary, to seek the optimum design for a network:

1. Start with the design for maximum heat recovery. The number of exchangers needed will be equal to or less than the number for maximum energy recovery.

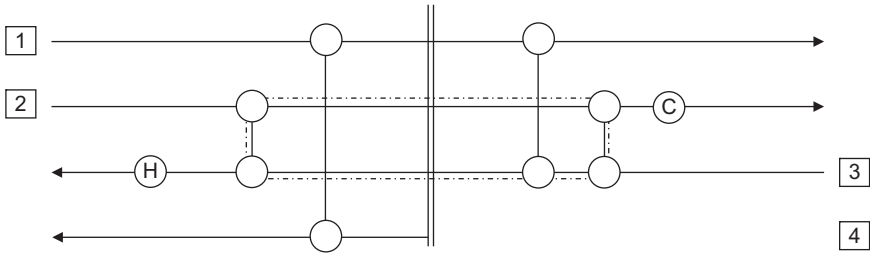


Fig. 3.26 Loop in network.

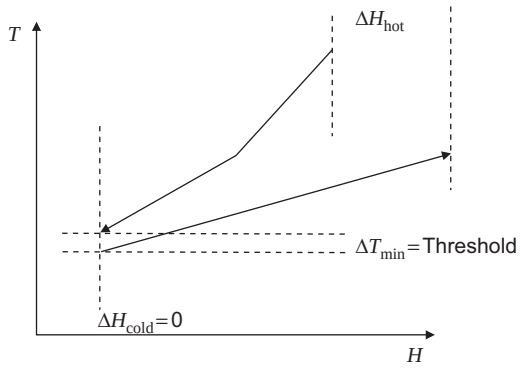


Fig. 3.27 Threshold problem.

2. Identify loops that cross the pinch. The design for maximum heat recovery will usually contain loops.
3. Starting with the loop with the least heat load, break the loops by adding or subtracting heat.
4. Check that the specified minimum temperature difference ΔT_{min} has not been violated. If the violation is significant, revise the design as necessary to restore ΔT_{min}. If the violation is small, it may not have much impact on the total annualized cost and can be ignored.
5. Estimate the capital and operating costs and the total annual cost.
6. Repeat the loop breaking and network revision to find the lowest-cost design.
7. Consider the safety, operability, and maintenance aspects of the proposed design.

3.5.5 Threshold problems

Problems that show the characteristic of requiring only either a hot utility or a cold utility (but not both) over a range of minimum temperature differences, from zero up to a threshold value, are known as *threshold problems*. A threshold problem is illustrated in Fig. 3.27.

To design the heat exchanger network for a threshold problem, it is normal to start at the most constrained point. The problem can often be treated as one-half of a problem exhibiting a pinch.

Threshold problems are often encountered in the process industries. A pinch can be introduced in such problems if multiple utilities are used, as in the recovery of heat to generate steam, or if the chosen value of ΔT_{min} is greater than the threshold value.

The procedures to follow in the design of threshold problems are discussed by Smith (2016) and Kemp (2007).

3.5.6 Determining utility consumption

Pinch analysis can be used to determine targets for process utility consumption. Initial targets for total hot and cold utility use can be calculated directly from the problem table algorithm or read from the composite curves. A more detailed breakdown of the utility needs can be determined from the initial heat exchanger network.

The following guidelines should be followed when using the pinch method to determine utility consumption targets:

1. Do not use cold utilities above the pinch temperature. This means that no process stream should be cooled from a temperature above the pinch temperature using a cold utility.
2. Do not use hot utilities below the pinch. This means no process stream should be heated from a temperature below the pinch temperature using a hot utility.
3. On either side of the pinch, maximize use of the cheapest utility first. Above the pinch this means use LP steam wherever possible before considering MP steam, then HP steam, hot oil, etc. Below the pinch, maximize use of cooling water before considering refrigeration.
4. If the process pinch is at a high temperature, consider boiler feed water preheat and steam generation as potential cold utility streams.
5. If the process pinch is at a low temperature, consider steam condensate and spent cooling water as hot streams.
6. If the process requires cooling to a very low temperature, consider using cascaded refrigeration cycles to improve the overall *COP*.
7. If the process requires heating to a very high temperature and a fired heater is needed, consider using the convective section heat either for process heating or for steam generation. For process control reasons, it may be necessary to operate the heater with process heating in the radiant section only, but the convective section heat is still available for use. In strict pinch terms, this heat can be used at any temperature above the pinch temperature, but in practice, convective section heat recovery is usually limited by the acid–gas dew point of the flue gas or other furnace design considerations (see Section 19.17).
8. If a process condition leads to the use of a more expensive utility, then consider process modifications that would make this unnecessary. For example, if a product must be cooled and sent to storage at 30 °C, the cooling cannot be carried out using cooling water and refrigeration must be used. The designer should question why 30 °C was specified for the storage. If it was because a vented tank was selected, then choosing a nonvented (floating roof) tank instead might allow the product to be sent to storage at 40 °C, in which case the refrigeration system could be eliminated.

Graphical methods and numerical approaches have been developed to assist in the optimal design of utility systems. For simple problems, these methods are not needed, as the heaters and coolers that have been identified in the heat exchange network can be assigned to the appropriate utility stream using the simple rules provided earlier. When a stream requires heating or cooling over a broad temperature range, the designer should consider whether it is cheaper to break the duty into several exchangers, each served by the appropriate utility for a given temperature range, or whether it makes more economic sense to use a single exchanger served by the hottest or coldest utility. The problem of placing multiple utilities is illustrated in Example 3.6.

3.5.7 Process integration: Integration of other process operations

The pinch technology method can give many other insights into process synthesis beyond the design of heat exchanger networks. The method can also be applied to the integration of other process units, such as separation columns, reactors, compressors and expanders, boilers, and heat pumps. The wider applications of pinch technology are discussed in the *Institution of Chemical Engineers Guide*, Kemp (2007), El-Halwagi (2006), and Smith (2016).

The techniques of process integration have been expanded for use in optimizing mass transfer operations and have been applied in waste reduction, water conservation, and pollution control; see El-Halwagi (2017) and Dunn and El-Halwagi (2003).

3.5.8 Computer tools for heat exchanger network design

Most pinch analysis in industry is carried out using commercial pinch analysis software. Programs such as Aspen HX-Net (Aspen Technology, Inc.), SUPERTARGET (Linnhoff March Ltd.), and UniSim ExchangerNet (Honeywell International, Inc.) allow the design engineer to plot composite curves, optimize ΔT_{min}, set targets for multiple utilities, and design the heat exchanger network.

Most of these programs are able to automatically extract stream data from process simulation programs, although great care should be taken to check the extracted data. There are many possible pitfalls in data extraction—for example, not recognizing changes in the *CP* of a stream or partial vaporization or condensation of a stream, any of which could lead to a kink in the stream *T-H* profile. See Smith (2016), Knopf (2012), Zhu (2014), or Kemp (2007) for more information on data extraction.

The commercial pinch technology tools also usually include automatic heat exchanger network synthesis features. The automatic synthesis methods are based on MINLP optimization of superstructures of possible exchanger options (see Chapter 12 for a discussion of MINLP methods). These tools can be used to arrive at a candidate network, but the optimization must be properly constrained so that it does not introduce a large number of stream splits and add a lot of small exchangers. Experienced designers seldom use automatic heat exchanger network synthesis methods, as it usually requires more effort to turn the resulting network into something practical than it would take to design a practical network manually. The NLP optimization capability of the software is widely used, though, for fine-tuning the network temperatures by exploitation of loops and stream split ratios.

Example 3.5

Determine the pinch temperatures and the minimum utility requirements for the streams set out in the following table for a minimum temperature difference between the streams of 20 °C. Devise a heat exchanger network to achieve the maximum energy recovery.

Stream Number	Type	Heat Capacity Flow Rate, kW/°C	Source Temp. °C	Target Temp. °C	Heat Load, kW
1	hot	40.0	180	40	5600
2	hot	30.0	150	60	1800
3	cold	60.0	30	180	9000
4	cold	20.0	80	160	1600

Solution

The problem table to find the minimum utility requirements and the pinch temperature can be built in a spreadsheet. The calculations in each cell are repetitive, and the formula can be copied from cell to cell using the cell copy commands. A spreadsheet template for the problem table algorithm is available in Microsoft Excel format in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793. The use of the spreadsheet is illustrated in Fig. 3.28 and is described here.

Company Name
Address

Project Name
Project Number Sheet 1 of 1

REV	DATE	BY	APVD	REV	DATE	BY	APVD

PROBLEM TABLE ALGORITHM

Form XXXXX-YY-ZZ

1. Minimum temperature approach

ΔT_{min} 20 °C

2. Stream data

Stream No.	Actual temperature (°C) Source	Target	Interval temperature (°C) Source	Target	Heat capacity flow rate *CP* (kW/°C)	Heat load (kW)
1	180	40	170	30	40	5600
2	150	60	140	50	30	2700
3	30	180	40	190	60	9000
4	80	160	90	170	20	1600
5						0
6						0
7						0
8						0

3. Problem table

Interval	Interval temp (°C)	Interval ΔT (°C)	Sum CP_c – sum CP_h (kW/°C)	d*H* (kW)	Cascade (kW)	(kW)
	190				0	2900
1	170	20	60	1200	–1200	1700
2	170	0	60	0	–1200	1700
3	140	30	40	1200	–2400	500
4	90	50	10	500	–2900	0
5	50	40	–10	–400	–2500	400
6	40	10	20	200	–2700	200
7	30	10	–40	–400	–2300	600
8						

Fig. 3.28 Problem table algorithm spreadsheet.

First calculate the interval temperatures for $\Delta T_{min} = 20\ ^\circ C$

$$\text{hot streams } T_{int} = T_{act} - 10\ ^\circ C$$

$$\text{cold streams } T_{int} = T_{act} + 10\ ^\circ C$$

	Actual temp. °C		Interval temp. °C	
Stream	**Source**	**Target**	**Source**	**Target**
1	180	40	170	30
2	150	60	140	50
3	30	180	40	190
4	80	160	90	170

In the spreadsheet this can be done by using an IF function to determine whether the source temperature is lower than the target temperature, in which case the stream is a cold stream and should have ΔT_{min} / 2 added.

Next rank the interval temperatures, ignoring any duplicated values. In the spreadsheet this is done using the LARGE function. Determine which streams occur in each interval. For a stream to be present in a given interval, the largest stream interval temperature must be greater than the lower end of the interval range, and the lowest stream interval temperature must also be greater than or equal to the lower end of the interval range. This can be calculated in the spreadsheet using IF, AND, and OR functions. Once the streams in each interval have been determined, it is possible to calculate the combined stream heat capacities. These calculations are not strictly part of the problem table, so they have been hidden in the spreadsheet in columns to the right of the table.

The sum of CP values for the cold streams minus that for the hot streams can then be multiplied by the interval ΔT to give the interval ΔH, and the interval ΔH values can be cascaded to give the overall heat flow. The amount of heat that must be put in to prevent the heat flow from becoming negative is the lowest value in the column, which can be found using the SMALL function. The final column then gives a cascade showing only positive values, with zero energy cascading at the pinch temperature.

In the last column 2900 kW of heat have been added to eliminate the negative values in the previous column, so the hot utility requirement is 2900 kW and the cold utility requirement, the bottom value in the column, is 600 kW.

The pinch occurs where the heat transferred is zero, that is, at interval number 4, interval temperature 90 °C.

So at the pinch hot streams will be at:

$$90 + 10 = 100\ ^\circ C$$

and the cold streams will be at:

$$90 - 10 = 80\ ^\circ C$$

Note that in the table both stream 1 and stream 4 had an interval temperature of 170 °C, which led to a duplicate line in the list of ranked interval temperatures. Strictly, this line could have been eliminated, but because it gave a zero value for the ΔT, it did not affect the calculation. The programming of the spreadsheet is a lot easier if duplicate temperatures are handled in this manner.

To design the network for maximum energy recovery, start at the pinch and match streams, following the rules on stream heat capacities for matches adjacent to the pinch. Where a match is made, transfer the maximum amount of heat.

The proposed network is shown in Fig. 3.29. The methodology followed in devising this network was as follows.

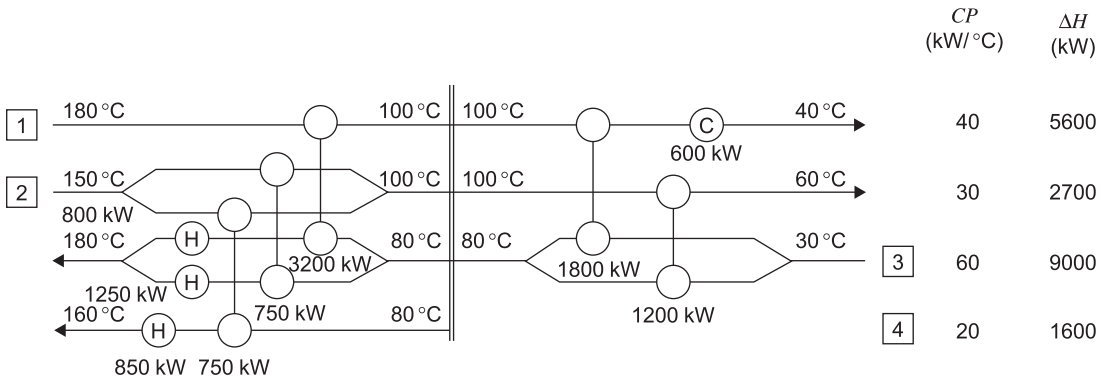


Fig. 3.29 Proposed heat exchanger network for Example 3.5.

Above pinch

1. $CP_h \leq CP_c$
2. Can match stream 1 or 2 with stream 3, but neither stream can match with stream 4. This creates a problem, because if we match stream 1 with 3, then stream 2 will not be able to make a match at the pinch. Likewise, if we match stream 2 with 3, then stream 1 will not be able to make a match at the pinch.
3. Check the heat available in bringing the hot streams to the pinch temperature.

$$\text{stream 1 } \Delta H = 40.0(180 - 100) = 3200 \text{ kW}$$

$$\text{stream 2 } \Delta H = 30.0(150 - 100) = 1500 \text{ kW}$$

4. Check the heat required to bring the cold streams from the pinch temperature to their target temperatures.

$$\text{stream 3 } \Delta H = 60.0(180 - 80) = 6000 \text{ kW}$$

$$\text{stream 4 } \Delta H = 20.0(160 - 80) = 1600 \text{ kW}$$

5. If we split stream 3 into two branches with *CP* of 40.0 and 20.0, then we can match the larger branch with stream 1 and transfer 3200 kW; that satisfies (ticks off) stream 1.
6. We now have two cold streams, both with *CP* of 20.0 and one hot stream (2) with *CP* of 30.0. We need to split stream 2 into two branches. As an initial guess, these can both have *CP* of 15.0. We can then match one branch of stream 2 with the smaller branch of 4 and transfer 750 kW, and the other branch with stream 3, also for 750 kW, which then ticks off stream 2.
7. Include a heater on the larger branch of stream 3 to bring it to its target temperature:

$$\Delta H_{hot} = 40(100) - 3200 = 800 \text{ kW}$$

8. Include a heater on the smaller branch of stream 3 to provide the balance of the heat required:

$$\Delta H_{hot} = 20(100) - 750 = 1250 \text{ kW}$$

9. Include a heater on stream 4 to provide the balance of the heat required:

$$\Delta H_{hot} = 1600 - 750 = 850 \text{ kW}$$

Check sum of heater duties = 800 + 1250 + 850 = 2900 kW = hot utility target.

Below pinch

9. $CP_h \geq CP_c$
10. Note that stream 4 starts at the pinch temperature so it cannot provide any cooling below the pinch.
11. Cannot match stream 1 or 2 with stream 3 at the pinch.
12. Split stream 3 to reduce *CP*. An even split will allow both streams 1 and 2 to be matched with the split streams adjacent to the pinch, so try this initially.
13. Check the heat available from bringing the hot streams from the pinch temperature to their target temperatures.

$$\text{stream 1 } \Delta H = 40.0(100 - 40) = 2400 \text{ kW}$$

$$\text{stream 2 } \Delta H = 30.0(100 - 60) = 1200 \text{ kW}$$

14. Check the heat required to bring the cold streams from their source temperatures to the pinch temperature:

$$\text{stream 3 } \Delta H = 60.0(80 - 30) = 3000 \text{ kW}$$

stream 4 is at the pinch temperature.

15. Note that stream 1 cannot be brought to its target temperature of 40 °C by full interchange with stream 3, as the source temperature of stream 3 is 30 °C, so ΔT_{min} would be violated. So transfer 1800 kW to one leg of the split stream 3.

16. Check the temperature at the exit of this exchanger:

$$\text{Temp out} = 100 - \frac{1800}{40} = 55^{\circ}\text{C, satisfactory}$$

17. Provide a cooler on stream 1 to bring it to its target temperature; the cooling needed:

$$\Delta H_{\text{cold}} = 2400 - 1800 = 600 \text{ kW}$$

18. Transfer the full heat load from stream 2 to the second leg of stream 3; this satisfies both streams.

Note that the heating and cooling loads, 2900 kW and 600 kW, respectively, match those predicted from the problem table.

Also note that to satisfy the pinch decomposition and the stream matching rules we ended up introducing a large number of stream splits. This is quite common in heat exchanger network design. None of the three split fractions was optimized, so substantial savings, as well as simplification of the network, could be possible. For example, loops exist between the branches of stream 3 and stream 1 and between the branches of stream 3 and stream 2. With the current split ratios, these loops cannot be eliminated, but with other ratios, it might be possible to eliminate one or two exchangers.

The introduction of multiple stream splits is often cited as a drawback of the pinch method. Stream splits can be problematic in process operation. For example, when an oil or other multicomponent stream is heated and partially vaporized, then the stream is a two-phase mixture. It is difficult to control the splitting of such streams to give the required flow rate in each branch. Experienced designers usually constrain the network to avoid multiple stream splits whenever possible, even if this leads to designs that have higher-than-minimum utility consumption.

Example 3.6

Determine the mix of utilities to use for the process introduced in Example 3.5 if the following utility streams are available:

Utility Stream	T_{supply} (°C)	T_{return} (°C)	Cost
MP steam (20 bar)	212	212	\$5.47/1000 lb
LP steam (6 bar)	159	159	\$4.03/1000 lb
Cooling water	30	40	\$0.10/1000 gal
Chilled water	10	20	\$4.50/GJ

Solution

From the solution to Example 3.5, we have the following heating and cooling duties that require utilities:

- Cooler on stream 1, duty 600 kW, to cool stream 1 from 55 °C to 40 °C
- Heater on large branch of stream 3, duty 800 kW, to heat from 160 °C to 180 °C
- Heater on small branch of stream 3, duty 1250 kW, to heat from 117.5 °C to 180 °C
- Heater on stream 4, duty 750 kW, to heat from 117.5 °C to 160 °C

It is obvious by inspection that if we are to maintain an approach temperature of 20 °C, then we will need to use MP steam and chilled water in at least some of the utility exchangers.

We can start by converting the utility costs into annual costs to provide a kW of heating or cooling based on an assumed 8000 hours per year of operation.

For MP steam at 20 bar:

- Heat of condensation (by interpolation in steam tables) ≈ 1889 kJ/kg
- 1 kW = 3600 × 8000 kJ/yr, therefore requires 3600 × 8000 / 1889 = 15.2 × 10^3 kg/y
- Annual cost per kW = 15.2 × 10^3 × 2.205 (lb/kg) × 5.47 (\$/1000 lb) /1000 = \$183 /y

Similarly for LP steam at 6 bar:

- Heat of condensation (by interpolation in steam tables) ≈ 2085 kJ/kg
- 1 kW = 3600 × 8000 kJ/yr, therefore requires 3600 × 8000 / 2085 = 13.8 × 10^3 kg/y
- Annual cost per kW = 13.8 × 10^3 × 2.205 (lb/kg) × 4.03 (\$/1000 lb) /1000 = \$123 /y

For cooling water with a cooling range of 10 °C

- 1 kW of cooling requires $CP = 1/10 = 0.1$ kW/°C
- Heat capacity of water ≈ 4.2 kJ/kg°C, so:
- Annual flow rate of cooling water per kW $= 0.1 \times 3600 \times 8000 / 4.2 = 686 \times 10^3$ kg/y
- 1000 gal of water = 3785 liters and has mass roughly 3785 kg, so:
- water flow rate $= 686 \times 10^3 / 3785 = 181.2$ thousand gallons per year, which has annual cost $0.1 \times 181.2 = \$18.1$ /y

For chilled water:

1 kW of cooling $= 3600 \times 8000 = 28.8 \times 10^6$ kJ/y $= 28.8$ GJ/y
So, annual cost $= 28.8 \times 4.50 = \$129.6$ /y

It is clearly cheaper to use LP steam rather than MP steam and to use cooling water instead of chilled water whenever it is feasible to do so.

Beginning with the design below the pinch, if we are to maintain a minimum temperature difference of 20 °C, then we cannot use cooling water below 30 + 20 = 50 °C. The lowest utility cost design would therefore use cooling water to cool stream 1 from 55 °C to 50 °C (duty 200 kW). A second cooler would then be needed to cool stream 1 from 50 °C to 40 °C using chilled water (duty 400 kW). The annual utility cost of this design would be 200(18.1) + 400(129.6) = $55,460.

It might reasonably be argued that the utility savings from using the minimum cost of coolant do not justify the capital cost of an extra exchanger. Two possible alternatives can be considered. If all of the cooling is carried out using chilled water, then the minimum temperature difference constraint is not violated and a single cooler of duty 600 kW can be used. The annual utility cost would be 600(129.6) = $77,760. The use of chilled water gives larger log-mean temperature difference in the cooler, so the total surface area required in this design is less than the sum of the areas needed for the two exchangers proposed earlier. The incremental operating cost would have to be traded against the capital cost savings. Alternatively, if we jettison the 20 °C minimum temperature difference and allow a 10 °C minimum temperature difference in the cooler, then we can cool stream 1 using only cooling water in a single cooler of duty 600 kW. The annual utility cost would be 600(18.1) = $10,860. The savings in operating cost would have to be traded against the increased capital cost that would result from having a lower log-mean temperature difference for this exchanger.

Turning now to the design above the pinch, LP steam cannot be used for heating any stream that is above a temperature of 159 − 20 = 139 °C. The minimum utility cost design would therefore use the following heaters:

- LP steam to heat stream 4 from 117.5 °C to 139 °C
- LP steam to heat the small branch of stream 3 from 117.5 °C to 139 °C
- MP steam to heat the small branch of stream 3 from 139 °C to 180 °C
- MP steam to heat the large branch of stream 3 from 160 °C to 180 °C
- MP steam to heat stream 4 from 139 °C to 160 °C

Again, although this design has the minimum utility cost, other designs may be more optimal when capital costs are also considered. For example, there is no reason why the two branches of stream 3 must be sent to separate MP steam heaters. These two heaters could be combined, even though that violates the rule of thumb about not mixing streams at different temperatures, as we are well away from the pinch and have already ensured maximum use of LP steam. This modification would reduce capital cost with no increase in operating cost, so would almost certainly be adopted. Another modification to consider would be to examine allowing a smaller minimum temperature difference for the heaters that use LP steam. This would increase LP steam use at the expense of more capital (reduced temperature difference in the exchangers) and so would require a trade-off between the additional capital and the energy cost savings.

Note that by introducing the lowest-cost utilities into the design we went from needing three heaters and one cooler in Fig. 3.29 to using two coolers and five heaters in the lowest-cost utility design. The introduction of multiple utilities almost always leads to an increase in the number of heat exchangers needed in a design, as well as the surface area requirements, and the energy cost savings must justify the resulting increase in capital cost.

3.6 Energy management in unsteady processes

The energy recovery approaches described earlier have been for steady-state processes, where the rate of energy generation or consumption did not vary with time. Batch and cyclic processes present multiple challenges for energy management. The designer must not only consider the amount of heat that must be added to or removed from the process but also the dynamics of heat transfer. Limitations on the rate of heat transfer often cause heating and cooling steps to become the rate-limiting steps in determining the overall cycle time. The sequential nature of batch operations can also reduce the possibilities for heat recovery by heat exchange unless multiple batches are processed in parallel and sequenced such that heat can be transferred from one batch to the next.

3.6.1 Differential energy balances

If a batch process is considered, or if the rate of energy generation or removal varies with time, it is necessary to set up a differential energy balance. For batch processes, the total energy requirements can usually be estimated by taking a single batch as the time basis for the calculation, but the maximum rate of heat generation must also be estimated to size any heat transfer equipment needed.

A generalized differential energy balance can be written as:

$$\text{Energy out} = \text{Energy in} + \text{generation} - \text{consumption} - \text{accumulation} \tag{3.8}$$

The energy in and energy out terms should include both heat transfer and convective heat flows, and the generation and consumption terms include heat of mixing, heat of reaction, etc. An unsteady-state mass balance must usually be solved simultaneously with the differential energy balance.

Most batch processing operations are carried out in the liquid phase in stirred tanks. In the simplest case, heat is only added or removed when the vessel is full, and the convective heat flows can be neglected. If there is no heat of reaction or mixing, then Equation 3.8 simplifies to:

$$\text{Rate of heat accumulation} = \text{rate of heat transfer into vessel} \tag{3.9}$$

$$MC_p \frac{dT}{dt} = UA\Delta T_m \tag{3.10}$$

where M = the mass contained in the vessel, kg
C_p = the specific heat capacity of the vessel contents, J/kg°C
T = temperature of the vessel contents, °C
t = time, s
U = the overall heat transfer coefficient, W/m^2°C
A = heat transfer area, m^2
ΔT_m = the mean temperature difference, the temperature driving force, °C

The mean temperature difference for heat transfer, ΔT_m, will generally be a function of the temperature of the vessel contents, T, as well as depending on the nature of the heating or cooling medium (isothermal or nonisothermal) and the type of heat transfer surface used. Batch tanks are usually heated or cooled using internal coils, jacketed vessels, or external heat exchangers. Heat transfer to vessels is discussed in more detail in Section 19.18.

In more complex cases, it is usually a good idea to set up a dynamic simulation model of the process. The use of dynamic simulation allows the designer to include additional heat source and sink terms such as losses to the environment. The designer can also use the dynamic model to investigate the interaction between the process, the heat transfer equipment, and the process control system, and hence to develop control algorithms that ensure rapid heating or cooling but do not cause excessive overshoot of the target temperature.

The application of differential energy balances to simple problems is illustrated in Examples 3.7 and 15.6.

3.6.2 Energy recovery in batch and cyclic processes

Most batch processes operate at relatively low temperatures, below 200 °C, where use of steam or hot oil will give high heat transfer rates for process heating. High heat transfer rates allow shorter heating times and enable use of internal coils and jacketed vessels, reducing the number of pieces of equipment in the plant. If the energy cost is a very small fraction of the total cost of production, then recovering heat from the process may not be economically attractive, as the resulting increase in capital cost will not be justified.

Many batch processes need cooling to temperatures that require some degree of refrigeration. Fermentation processes are often operated at temperatures below 40 °C, where use of cooling water can be problematic and chilled water or other refrigerants are used instead. Food processes often require refrigeration or freezing of the product. Recovery of "cooling" from chilled streams is not possible when the product must be delivered in chilled form.

Three of the most commonly used methods for recovering heat in batch and cyclic processes are described next. Energy optimization in batch plants has been the subject of much research and is discussed in more detail in the papers by Vaselenak et al. (1986), Kemp and Deakin (1989), and Lee and Reklaitis (1995) and the books by Smith (2016), Kemp (2007), and Majozi (2010).

Semicontinuous operation

The simplest approach to allow some degree of heat recovery in a batch process is to operate part of the plant in a continuous mode. The use of intermediate accumulation tanks can allow sections of the plant to be fed continuously or to accumulate product for batching into other operations.

Semicontinuous operation is often deployed for feed sterilizers and pasteurizers in food processing and fermentation plants. In a pasteurization operation, the feed must be heated to a target temperature, held at that temperature for long enough to kill unwanted species that may be present in the feed, and then cooled to the process temperature. The high-temperature residence time is usually obtained by passing the process fluid through a steam-traced or well-insulated pipe coil. The initial heating of the feed can be accomplished by heat exchange, with the hot fluid leaving the coil, allowing the use of a smaller steam heater to reach the target temperature, as shown in Fig. 3.30. This design is common in food processing plants, but care must be taken to ensure that there is no leakage across the heat exchanger, which could potentially lead to contamination of the "sterile" feed with components from the raw feed.

Another situation where semicontinuous operation is often adopted is in the separation section of a batch plant. Some energy-intensive separations such as distillation and crystallization are easier to control to high recovery and tight product specifications when operated in continuous mode. In these cases a surge tank can feed the continuous section of the plant, and typical heat recovery schemes such as feed-bottoms heat exchange can be considered.

If a batch plant is designed so that batches are transferred from one vessel to another (as opposed to undergoing successive steps in the same vessel), then heat can be transferred between streams as they are pumped from one vessel to the next. During the pumping operation the flow is at a pseudo-steady state, and a heat exchanger between two streams behaves the same as a heat exchanger in a continuous plant. Fig. 3.31 shows such an arrangement in which a hot stream flows from vessel *R1* to vessel *R2*, while a cold stream flows from vessel *R3* to vessel *R4*. The flowing streams exchange heat in a heat exchanger that is shown as being countercurrent, but could equally well be cross-flow or co-current if the temperatures were suitable. This arrangement is sometimes referred to as a *"counter-current" heat integration*, although it should be stressed that the exchanger can be co-current or cross-flow.

When stream-to-stream heat transfer is used, a high degree of heat recovery can be obtained. The exchanger will perform well and maintain roughly constant stream outlet temperatures during the period when the vessels are being pumped out. When the liquid level in the vessels becomes too low for pump operation, the flow rates in the exchanger become too low for the exchanger to function effectively. If batch-to-batch contamination is not important and there are no safety hazards, product quality issues, or fouling concerns, then the exchanger can be isolated ("blocked in") while the remaining tank contents are drained through bypass lines, and the exchanger is then ready to be reused when tanks *R1* and *R3* are again ready to be drained. In the case where batch-to-batch

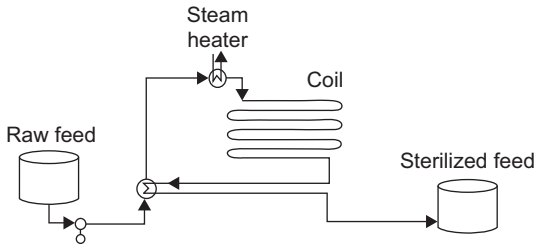


Fig. 3.30 Heat integration of feed sterilization system.

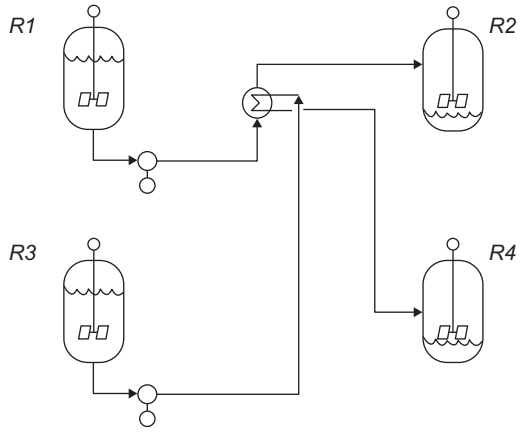


Fig. 3.31 Stream-to-stream ("counter-current") heat integration of batch vessels.

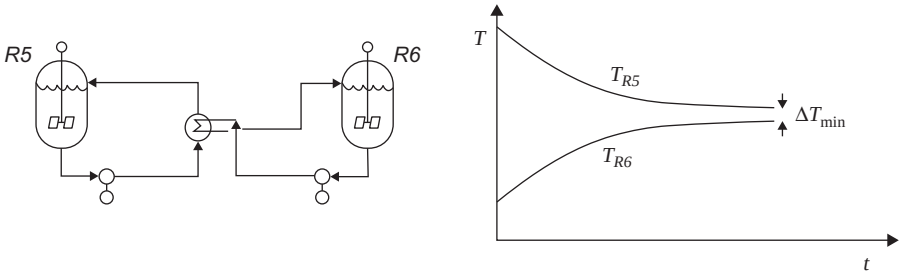


Fig. 3.32 Tank-to-tank ("co-current") heat integration of batch vessels.

mixing is not desired or where there are other reasons why the exchanger cannot be left full of process fluid, provision must be made to flush, drain, and clean the exchanger once the upstream tanks are empty.

Sequencing multiple batches

If a plant contains several batches that are undergoing different steps of a process at the same time, or if several different batch plants are grouped close to each other, then the batches can sometimes be sequenced so that heat can be transferred from one batch to another.

Suppose a batch process contains the steps of heating reagents, reacting them at a desired temperature and then cooling the products before sending them for further processing. If two reactors are used, a heat exchanger can be employed to exchange heat from the reactor that is being cooled to the reactor that is being heated. For example, in Fig. 3.32, hot fluid from vessel *R5* is pumped through an exchanger, where it transfers heat to cold fluid that is pumped from vessel *R6*. The fluid from each vessel is returned to the vessel that it came from. The heat exchanger in Fig. 3.31 is shown as being counter-current, but co-current or cross-flow heat exchange could be used if the temperatures were appropriate.

The graph on the right of Fig. 3.32 is a schematic of the temperature−time profile for both vessels. As time progresses, they become closer in temperature and would eventually reach thermal equilibrium. In practice, it is usually not economic to run the exchanger for very long times, and heat transfer is stopped when an acceptable minimum temperature difference between the vessels is reached, shown as ΔT_{min} in the figure. Tank-to-tank heat transfer does not allow as efficient heat recovery as stream-to-stream, as the hottest temperatures in the hot tank are matched with the coldest temperatures in the cold tank, as they would be in a co-current heat exchanger; hence Vaselenak et al. (1986) named this type of batch heat integration "co-current" heat integration. It should again be stressed that the heat exchanger is usually designed to be counter-current or cross-flow.

An improvement on this scheme is to use stream-to-tank heat transfer, shown in Fig. 3.33, in which a stream that is transferred from one vessel to another exchanges heat with a stream that is returned to the tank from which it originated. In Fig. 3.33, hot fluid flows from *R7* to *R8* and transfers heat to a cold stream that is pumped from *R9* and returned to *R9*. The graph on the right of Fig. 3.33 is a schematic of the temperature behavior of *R9*, *R8*, and the location marked as *A* on the line entering *R8*. The temperature of the cold fluid in *R9* increases over

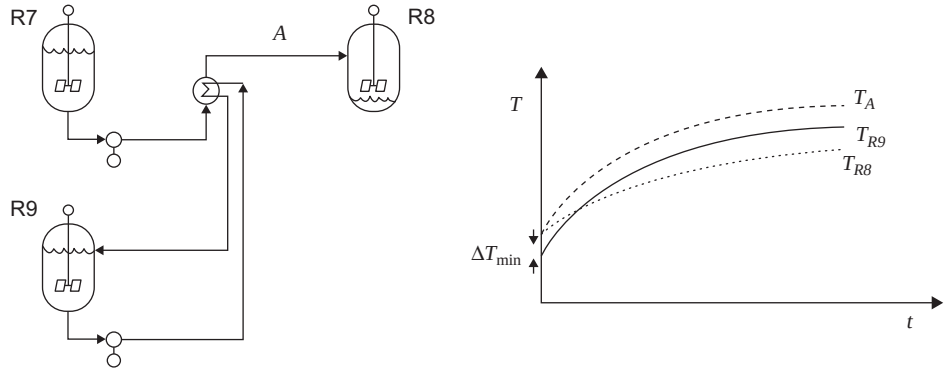


Fig. 3.33 Stream-to-tank ("co-current/countercurrent") heat integration of batch vessels.

time as heat is transferred to it. The temperature at *A* is the temperature of the hot fluid at the exit of the heat exchanger. The heat exchanger will usually be designed to pinch at the cold end, because the recirculating flow from *R9* can be much greater than the pump-out flow from *R7*. Consequently, the temperature at *A* will be equal to the temperature in *R9* plus the temperature approach of the heat exchanger, and so the temperature at *A* has a profile offset above the *R9* temperature profile. The temperature in *R8* is the time-averaged integral of the temperature of the feed to the vessel (i.e., the time-averaged integral of the temperature at *A*). Although the fluid entering *R8* becomes hotter with time, it is mixed with an accumulating volume of colder fluid, so the temperature in *R8* does not increase so rapidly as the temperature in *R9*, and *R8* can even be colder than *R9* when the heat transfer is complete. This process is therefore intermediate in terms of thermal efficiency between tank-to-tank heat transfer and stream-to-stream heat transfer. It is sometimes known as *"co-current/counter-current" heat integration*. The derivation of the equations needed to accurately describe the temperature profiles for this arrangement is given by Vaselenak et al. (1986).

When tank-to-tank or tank-to-stream heat transfer is selected, care must be taken to ensure that the heat exchanger doesn't cause problems when not in use. If the designer anticipates that there could be problems with fouling, corrosion, batch-to-batch contamination, product degradation, safety issues, or any other issue with leaving the exchanger filled, then the design must include means to drain, flush, and clean the exchanger between batches.

When considering the use of stream-to-stream, stream-to-tank, or tank-to-tank heat transfer in a batch process, the designer must ensure that the batch schedules allow both streams to be available at the same time and for a sufficient time to accomplish the desired heat recovery. When draining, flushing, and cleaning of the heat exchanger are necessary, these steps must also be taken into account. For a process that handles multiple batches simultaneously or a site with multiple batch plants, the resulting scheduling problem becomes too large to optimize by hand and numerical methods must be used. See Vaselenak et al. (1986), Kemp and Deakin (1989), and Lee and Reklaitis (1995) for approaches to solving such problems.

Indirect heat recovery

An alternative method of heat recovery that can be used in batch processing is to recover heat indirectly through the utility system or using a heat storage system. Although less thermally efficient than process-to-process heat recovery, this method eliminates problems from sequencing of operations.

In indirect heat recovery, heat from a hot process stream is transferred to a utility stream, such as a reservoir of heat transfer fluid. The heat transfer fluid can then be used for heating elsewhere in the process. Indirect heat recovery can be used in any of the flow schemes described earlier, but in all cases the use of an intermediate stream will reduce the thermal efficiency and the amount of heat that can be recovered. Heat storage systems can only be used when there is a large enough temperature difference between the process heat source and process heat sink to allow for the thermal inefficiency of transfer of heat to the storage medium, cooling losses during storage, and transfer of heat to the process heat sink.

Example 3.7 Differential energy balance

In the batch preparation of an aqueous solution, the water is first heated to 80 °C in a jacketed, agitated vessel; 1000 Imp. gal. (4545 kg) is heated from 15 °C. If the jacket area is 300 ft^2 (27.9 m^2) and the overall heat transfer coefficient can be taken as 50 Btu ft^{-2} h^{-1} $°F^{-1}$ (285 W m^{-2} K^{-1}), estimate the heating time. Steam is supplied at 25 psig (2.7 bar).

Solution

The rate of heat transfer from the jacket to the water will be given by Equation 3.10:

$$MC_p \frac{dT}{dt} = UA\Delta T_m \tag{3.10}$$

Because steam is used as the heating medium, the hot side is isothermal and we can write:

$$\Delta T_m = T_s - T$$

where T_s = the steam saturation temperature.
Integrating:

$$\int_0^{t_B} dt = \frac{MC_p}{UA} \int_{T_1}^{T_2} \frac{dT}{(T_s - T)}$$

Batch heating time, t_B:

$$t_B = -\frac{MC_p}{UA} \ln \frac{T_s - T_2}{T_s - T_1}$$

For this example

$$MC_p = 4.18 \times 4545 \times 10^3 \text{JK}^{-1}$$
$$UA = 285 \times 27 \text{ WK}^{-1}$$
$$T_1 = 15°\text{C}, T_2 = 80°\text{C}, T_s = 130°\text{C}$$
$$t_B = -\frac{4.18 \times 4545 \times 10^3}{285 \times 27.9} \ln \frac{130 - 80}{130 - 15}$$
$$= 1990\text{s} = 33.2 \text{ min}$$

In this example the heat capacity of the vessel and the heat losses have been neglected for simplicity. They would increase the heating time by 10% to 20%.

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3.8 Nomenclature

		Dimensions in $MLT\theta$
A	Area	L^2
CP	Stream heat capacity flow rate	$ML^2T^{-2}\theta^{-1}$
CP_c	Stream heat capacity flow rate, cold stream	$ML^2T^{-2}\theta^{-1}$
CP_h	Stream heat capacity flow rate, hot stream	$ML^2T^{-2}\theta^{-1}$
C_p	Specific heat at constant pressure	$L^2T^{-2}\theta^{-1}$
ΣCP_c	Sum of heat capacity flow rates of cold streams	$ML^2T^{-2}\theta^{-1}$
ΣCP_h	Sum of heat capacity flow rates of hot streams	$ML^2T^{-2}\theta^{-1}$
COP	Coefficient of performance for a refrigeration cycle	—
COP_h	Coefficient of performance for a heat pump	—
dH_b	Boiler heating rate	$L^{-2}T^2$
H	Enthalpy	ML^2T^{-2}
ΔH	Change in enthalpy	ML^2T^{-2}
ΔH_{cold}	Heat transfer from cold utility	ML^2T^{-3}
ΔH_{ex}	Heat transfer in exchanger	ML^2T^{-3}
ΔH_{hot}	Heat transfer from hot utility	ML^2T^{-3}
ΔH_n	Net heat required in nth interval	ML^2T^{-3}

(Continued)

		Dimensions in $MLT\theta$
ΔH_{xp}	Cross-pinch heat transfer	ML^2T^{-3}
$-\Delta H^\circ_c$	Standard heat of combustion	L^2T^{-2}
ΔH°_f	Standard enthalpy of formation	L^2T^{-2}
h_g	Specific enthalpy of steam	L^2T^{-2}
L'	Number of internal loops in network	—
M	Mass	M
m	Mass flow rate	MT^{-1}
N	Number of cold streams, heat exchanger networks	—
N'	Number of streams	—
P_{BFW}	Price of boiler feed water	$\$M^{-1}$
P_F	Price of fuel	$\$M^{-1}L^{-2}T^2$
P_{HPS}	Price of high-pressure steam	$\$M^{-1}$
S	Number of independent branches	—
s_g	Specific entropy	$L^2T^{-2}\theta^{-1}$
T	Temperature, absolute	θ
T_1	Initial temperature	θ
T_2	Final temperature	θ
T_{act}	Actual stream temperature	θ
T_c	Condenser temperature	θ
T_e	Evaporator temperature	θ
T_{int}	Interval temperature	θ
T_n	Temperature in nth interval	θ
T_{pinch}	Pinch temperature	θ
T_{return}	Return temperature for utility	θ
T_s	Source temperature	θ
T_{supply}	Supply temperature for utility	θ
T_s	Steam saturation temperature	θ
T_t	Target temperature	θ
ΔT_m	Mean temperature difference	θ
ΔT_{min}	Minimum temperature difference (minimum approach) in heat exchanger	θ
ΔT_n	Interval temperature difference	θ
t	Time	T
t_B	Batch heating time	T
U	Overall heat transfer coefficient	$MT^{-3}\theta^{-1}$
Z_{min}	Minimum number of heat exchangers in network	—
η_B	Boiler efficiency	—

3.9 Problems

3.1. A process heater uses Dowtherm A heat transfer fluid to provide 850 kW of heat. Estimate the annual operating cost of the heater if the Dowtherm evaporator is 80% efficient and the price of natural gas is $4.60/MMBtu. Assume 8000 operating hours per year.

3.2. A site steam system consists of HP steam at 40 bar, MP steam at 18 bar, and LP steam at 3 bar. If natural gas costs $3.50/MMBtu and electricity is worth $0.07/kWh, estimate the cost of steam at each level in $/metric ton.

3.3. Make a rough estimate of the cost of steam per ton produced from a packaged boiler with 10,000 kg per hour of steam required at 15 bar. Natural gas will be used as the fuel, with calorific value 39 MJ/m^3 (roughly 1 MMBtu/1000 scf). Take the boiler efficiency as 80%. No condensate will be returned to the boiler.

3.4. A crystallization process requires operation at $-5\ ^\circ C$. The refrigeration system can reject heat to cooling water that is available at 35 °C. If a single refrigeration cycle has an efficiency of 60% of Carnot cycle performance, estimate the cost of providing 1 kW of cooling to this process using a single-stage cycle and using a cascaded-two stage cycle (in which the colder cycle rejects heat to the warmer cycle). Electricity costs $0.07/kWh, and the cost of cooling water can be neglected.

3.5. A gas produced as a by-product from the carbonization of coal has the following composition, mole percent: carbon dioxide 4, carbon monoxide 15, hydrogen 50, methane 12, ethane 2, ethylene 4, benzene 2, balance

nitrogen. Using the data given in Appendix C (available online at www.elsevier.com/books-and-journals/book-companion/9780128211793), calculate the gross and net calorific values of the gas. Give your answer in MJ/m^3 at standard temperature and pressure.

3.6. Determine the pinch temperature and the minimum utility requirements for the process set out here. Take the minimum approach temperature as 15 °C. Devise a heat exchanger network to achieve maximum energy recovery.

Stream Number	Type	Heat capacity kW/°C	Source Temp. °C	Target Temp. °C
1	Hot	13.5	180	80
2	Hot	27.0	135	45
3	Cold	53.5	60	100
4	Cold	23.5	35	120

3.7. Determine the pinch temperature and the minimum utility requirements for the process set out here. Take the minimum approach temperature as 15 °C. Devise a heat exchanger network to achieve maximum energy recovery.

Stream Number	Type	Heat capacity kW/°C	Source Temp. °C	Target Temp.°C
1	Hot	10.0	200	80
2	Hot	20.0	155	50
3	Hot	40.0	90	35
4	Cold	30.0	60	100
5	Cold	8.0	35	90

3.8. To produce a high-purity product two distillation columns are operated in series. The overhead stream from the first column is the feed to the second column. The overhead from the second column is the purified product. Both columns are conventional distillation columns fitted with reboilers and total condensers. The bottom products are passed to other processing units, which do not form part of this problem. The feed to the first column passes through a preheater. The condensate from the second column is passed through a product cooler. The duty for each stream is summarized here:

No.	Stream	Type	Source Temp. °C	Target Temp. °C	Duty, kW
1	Feed preheater	cold	20	50	900
2	First condenser	hot	70	60	1350
3	Second condenser	hot	65	55	1100
4	First reboiler	cold	85	87	1400
5	Second reboiler	cold	75	77	900
6	Product cooler	hot	55	25	30

Find the minimum utility requirements for this process, for a minimum approach temperature of 10 °C.

Note: The stream heat capacity is given by dividing the exchanger duty by the temperature change.

3.9. At what value of the minimum approach temperature does the problem in Example 3.5 become a threshold problem? Design a heat exchanger network for the resulting threshold problem. What insights does this give into the design proposed in Example 3.5?

CHAPTER

4

Process simulation

KEY LEARNING OBJECTIVES

- How to use commercial process simulation software to build a process heat and material balance model
- How to select thermodynamic models for prediction of phase equilibrium and stream properties
- How to use user-specified models and components when the simulator does not have what you need
- How to converge flowsheets that include recycles and overcome convergence problems
- How to optimize converged flowsheets

4.1 Introduction

This chapter addresses the use of process simulation tools in developing an overall process mass and energy balance. A process flow diagram or flowsheet typically includes material balances made over the complete process and each individual unit. Energy balances are also made to determine the energy flows and the utility requirements.

Most flowsheet calculations are carried out using commercial process simulation programs. The process simulation programs contain models for most unit operations as well as thermodynamic and physical property models. All the commercial programs feature some level of custom modeling capability that allows the designer to add models for nonstandard operations.

Many companies developed proprietary flowsheeting programs between 1960 and 1980. The cost of maintaining and updating proprietary software is high; consequently, very few of the proprietary flowsheeting programs are still in use, and most companies now rely entirely on commercially available software. Each of the commercial process simulation programs has its own unique idiosyncrasies, but they share many common features. The discussion in this chapter addresses general problems of process simulation and flowsheeting rather than software-specific issues. The latter are usually thoroughly documented in the user manuals and online help that come with the software. Examples have been provided in this chapter using both Aspen Plus (Aspen Technology, Inc.) and UniSim Design Suite (Honeywell International, Inc.). UniSim Design is based on the Hysys software that was originally developed by Hyprotech Ltd. and is now owned and licensed by Honeywell.

Cyclic and batch process operations that do not run at steady state require dynamic simulation models. Several of the steady-state process simulation programs can be modified to run as dynamic simulators. Specialized programs have also been developed for batch processing, such as SuperPro Batch Designer, which has many features tailored to the simulation of biological processes. Simulation of batch processes is discussed in Section 4.9.

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Because flowsheeting is usually carried out using computer programs, it is necessary for the design engineer to have a good understanding of how to set up and solve computer models. The flowsheet model that is solved on the computer to generate a mass and energy balance is often not an exact representation of the process flow diagram. The designer may need to use combinations of simulation library models and user models to capture the performance of process equipment. Spreadsheet or hand calculations are also often helpful in setting up process simulation models and providing good initial estimates so as to accelerate convergence.

4.2 Process simulation programs

The most commonly used commercial process simulation programs are listed in Table 4.1. Most of these programs can be licensed by universities for educational purposes at nominal cost.

Detailed discussion of the features of each of these programs is beyond the scope of this book. For a general review of the requirements, methodology, and application of process simulation programs, the reader is referred to the books by Husain (1986), Wells and Rose (1986), Leesley (1982), Benedek (1980), and Westerberg et al. (1979). The features of the individual programs are described in their user manuals and online help. Two of these simulators have been used to generate the examples in this chapter: Aspen Plus (v.11.1) and UniSim Design (R360.1). More recent versions of these programs are now available with additional features, but the screen appearance has not changed significantly since the examples were developed.

Process simulation programs can be divided into two basic types:

Sequential-modular programs, in which the equations describing each process unit (module) are solved module by module in a stepwise manner. Iterative techniques are then used to solve the problems arising from the recycle of information.

Simultaneous (also known as *equation-oriented*) programs, in which the entire process is described by a set of equations and the equations are solved simultaneously, not stepwise as in the sequential approach. Simultaneous programs can simulate the unsteady-state operation of processes and equipment and can give faster convergence when multiple recycles are present.

TABLE 4.1 Simulation packages

Name	Type	Source	Internet address www.—
Aspen Plus	steady-state	Aspen Technology Inc. Ten Canal Park Cambridge, MA 02141-2201, USA	Aspentech.com
CHEMCAD	steady-state	2901 Wilcrest, Suite 305 Houston, TX 77042 USA	Chemstations.net
DESIGN II	steady-state	WinSim Inc. P.O. Box 1885 Houston, TX 77251-1885, USA	Winsim.com
HYSYS	steady-state and dynamic	Aspen Technology Inc. Ten Canal Park Cambridge, MA 02141-2201, USA	Aspentech.com
PRO/II and DYNSIM	steady-state and dynamic	SimSci-Esscor 5760 Fleet Street Suite 100, Carlsbad, CA 92009, USA	Simsci.com
UniSim Design	steady-state and dynamic	Honeywell 300-250 York Street London, Ontario N6A 6K2, Canada	Honeywell.com

Note: Contact the website to check the full features of the most recent versions of the programs.

In the past, most simulation programs available to designers were of the sequential-modular type. They were simpler to develop than the equation-oriented programs and required only moderate computing power. The modules are processed sequentially, so essentially only the equations for a particular unit are in the computer memory at one time. Also, the process conditions, temperature, pressure, flow rate, etc., are fixed in time. With the sequential modular approach, computational difficulties can arise due to the iterative methods used to solve recycle problems and obtain convergence. A major limitation of sequential modular simulators is the inability to simulate the dynamic, time-dependent behavior of a process.

Simultaneous dynamic simulators require appreciably more computing power than steady-state simulators to solve the thousands of differential equations needed to describe a process, or even a single item of equipment. With the development of fast, powerful computers, this is no longer a restriction. By their nature, simultaneous programs do not experience the problems of recycle convergence inherent in sequential simulators; however, as temperature, pressure, and flow rate are not fixed and the input of one unit is not determined by the calculated output from the previous unit in the sequence, simultaneous programs demand more computer time. This has led to the development of hybrid programs in which the steady-state simulator is used to generate the initial conditions for the equation-oriented or dynamic simulation.

The principal advantage of simultaneous, dynamic simulators is their ability to model the unsteady-state conditions that occur at start-up and during fault conditions. Dynamic simulators are being increasingly used for safety studies and in the design of control systems, as discussed in Section 4.9.

The structure of a typical simulation program is shown in Fig. 4.1.

The program consists of:

1. A main executive program that controls and keeps track of the flowsheet calculations and the flow of information to and from the subroutines.
2. A library of equipment performance subroutines (modules) that simulate the equipment and enable the output streams to be calculated from information on the inlet streams.
3. A data bank of physical properties. To a large extent, the utility of a sophisticated flowsheeting program depends on the comprehensiveness of the physical property data bank. The collection of the physical property data required for the design of a particular process and its transformation into a form suitable for a particular flowsheeting program can be very time consuming.
4. Subroutines for thermodynamics, such as the calculation of vapor–liquid equilibrium and stream enthalpies.
5. Subprograms and data banks for equipment sizing and costing. Process simulation programs enable the designer to consider alternative processing schemes, and the cost routines allow quick economic comparisons to be made. Some programs include optimization routines. To make use of a costing routine, the program must be capable of producing at least approximate equipment designs.

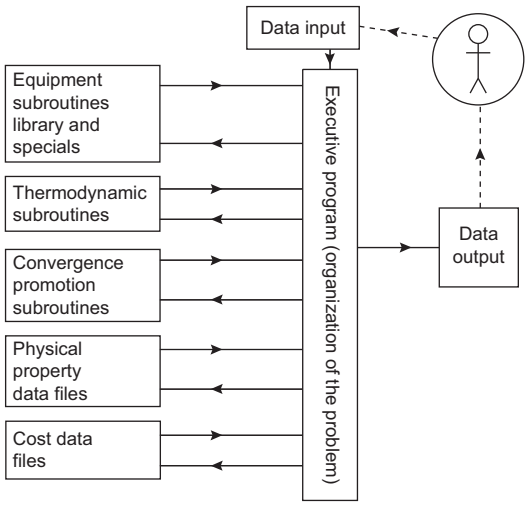


FIG. 4.1 A typical simulation program.

In a sequential-modular program, the executive program sets up the flowsheet sequence, identifies the recycle loops, and controls the unit operation calculations, while interacting with the unit operations library, physical property data bank, and the other subroutines. The executive program also contains procedures for the optimum ordering of the calculations and routines to promote convergence.

In an equation-oriented simulator, the executive program sets up the flowsheet and the set of equations that describe the unit operations and then solves the equations using data from the unit operations library and the physical property data bank and calling on the file of thermodynamics subroutines.

All process simulators use graphical user interfaces to display the flowsheet and facilitate the input of information to the package. The entry of data is usually intuitive to anyone familiar with the Microsoft Windows operating systems.

4.3 Specification of components

The first step in building a process simulation is usually establishing the chemical basis for the model. This consists of choosing the components that will be included in the mass balance and deciding which models to use for the prediction of physical properties and phase equilibrium. This section focuses on the selection of suitable components; the selection of physical property models is discussed in Section 4.4.

4.3.1 Pure components

Each of the commercial process simulation programs contains a large data bank of pure component compounds. Most of the pure components are organic compounds, but inorganic compounds and electrolytes are also included.

The fact that a pure component is listed in a simulator data bank does not guarantee that any of the properties given for that component are based on measured data. If the properties of a compound are critical to process performance, then the scientific literature should be consulted to confirm that the values used in the simulation are realistic.

The most important decision when building a pure component model is choosing the right number of components. The design engineer needs to consider carefully which components will have a significant impact on process design, operation, and economics. If too few components are used, the model will be inadequate for process design, as it will not correctly predict the performance of reactors and separation equipment. Conversely, if too many components are used, the model can become difficult to converge, particularly if there are multiple recycles in the design.

Some guidelines to keep in mind when building a component list include:

1. Always include any component that has a specified limit in any of the products if that component is present in any of the feeds or could be formed in the process. This is critical to determining whether the separations are meeting product specifications.
2. Always include any component that has a specified limit in any of the feeds. These components can be a source of by-products or can act as catalyst or enzyme inhibitors. They must be tracked to ensure that they do not accumulate in the process or make it difficult to meet product specifications. In some cases, an additional separation may be needed to remove a feed contaminant.
3. Always include components that are expected to be formed in side reactions or consecutive reactions. It is important to understand where these components will accumulate or leave the process, even if their yield is not yet known.
4. Always include any compounds that are expected to be present and are known to have significant health, safety, or environmental concerns, such as compounds with high toxicity or explosivity, known carcinogens, or listed hazardous air pollutants (see Chapter 10). These compounds must be tracked to make sure that they do not reach unsafe levels in any stream and to understand where they might be released to the environment.
5. Usually include any compound that might be present at a mass or mole fraction greater than 2% in any stream in the process.
6. Do not include isomers unless the process specifically requires distinction between isomers (for example, if the process is selective for one isomer, gives different products for different isomers, or is designed to separate isomers). Considering all of the possible isomers of organic compounds becomes combinatorically explosive at high carbon numbers. For fuels and bulk petrochemical processes that are carried out at relatively high temperatures, it is often reasonable to assume an equilibrium distribution of isomers. For fine chemical and

pharmaceutical processes, it is usually important to track isomers separately, particularly enantiomers, as the desired product is often only one of the isomers.

In general, pure component models solve more efficiently with fewer than about 40 components. If the number of components becomes too large and there are many recycles, it may be necessary to build two models. The first is a high-level model that contains only the main bulk components. This model is then used to initialize a second, more detailed model that has the full component list.

4.3.2 Pseudocomponents

Pseudocomponents (hypocomponents) are components created by the simulator to match the boiling curves of petroleum mixtures.

Crude oil; fuels such as gasoline, kerosene, and diesel; and most intermediate streams in an oil refinery consist of many different hydrocarbon compounds. The number of possible hydrocarbon isomers present depends on the carbon number, and both increase with boiling range. For diesel, crude oil, and heavy fuel oils, the number of possible compounds can be from 10^4 to $>10^6$. At the time of writing, there is no analytical method that can uniquely identify all of these compounds, so it would be impossible to include them all in a model even if the resulting model could be solved. Instead, a large number of possible compounds with boiling points in a given range are "lumped" together and represented by a single pseudocomponent with a boiling point in the middle of that range. A set of 10 to 30 pseudocomponents can then be fitted to any petroleum assay and used to model that oil.

Pseudocomponent models are useful for oil fractionation and blending problems. They can also be used to characterize heavy products in some chemical processes, such as ethane cracking. Pseudocomponents are treated as inert in most of the reactor models, but they can be converted or produced in yield shift reactors (see Section 4.5.1).

Some of the commercial simulation programs use a standard default set of pseudocomponents and fit the composition of each to match a boiling curve of the oil that is entered by the user. This can sometimes lead to errors when predicting ASTM D86 or D2887 curves for products from a feed that has been defined based on a true boiling point (TBP) curve or when making many subcuts or cuts with tight distillation specifications. It is often better to work back from the product distillation curves and add extra pseudocomponents around the cut points to make sure that the recoveries and 5% and 95% points on the product distillation curves are predicted properly. All of the simulators have the option to add pseudocomponents to the default set or use a user-generated curve.

4.3.3 Solids and salts

Most chemical and pharmaceutical processes involve some degree of solids handling. Examples of solids that must be modeled include:

- Components that are crystallized for separation, recovery, or purification
- Pharmaceutical products that are manufactured as powders or tablets
- Insoluble salts formed by the reaction of acids and bases or other electrolytes
- Hydrates, ice, and solid carbon dioxide that can form in cryogenic processes
- Cells, bacteria, and immobilized enzymes in biological processes
- Pellets or crystals of polymer formed in polymerization processes
- Coal and ash particles in power generation
- Catalyst pellets in processes in which the catalyst is fluidized or transported as a slurry
- Mineral salts and ores that are used as process feeds
- Fertilizer products
- Fibers in paper processing

Some solid phase components can be characterized as pure components and can interact with other components in the model through phase and reaction equilibrium. Others, such as cells and catalysts, are unlikely to equilibrate with other components, although they can play a vital role in the process.

In Aspen Plus, solid components are identified as different types. Pure materials with measurable properties such as molecular weight, vapor pressure, and critical temperature and pressure are known as *conventional solids* and are present in the MIXED substream with other pure components. They can participate in any of the phase or reaction equilibria specified in any unit operation. If the solid phase participates only in reaction equilibrium but not in phase equilibrium (for example, when the solubility in the fluid phase is known to be very low), then it is called a

conventional inert solid and is listed in a substream CISOLID. If a solid is not involved in either phase or reaction equilibrium, then it is a nonconventional solid and is assigned to substream NC. Nonconventional solids are defined by attributes rather than molecular properties and can be used for coal, cells, catalysts, bacteria, wood pulp, and other multicomponent solid materials.

In UniSim Design, nonconventional solids can be defined as hypothetical components (see Section 4.3.4). The solid phases of pure components are predicted in the phase and reaction equilibrium calculations and do not need to be identified separately.

Many solids-handling operations have an effect on the particle size distribution (PSD) of the solid phase. The PSD can also be an important product property. Aspen Plus allows the user to enter a PSD as an attribute of a solid substream. In UniSim Design, the PSD is entered on the "PSD Property" tab, which appears under "worksheet" on the stream editor window for any stream that contains a pure or hypothetical solid component. Unit operations such as yield shift reactor, crusher, screen, cyclone, electrostatic precipitator, and crystallizer can then be set up to modify the PSD, typically by using a conversion function or a particle capture efficiency in each size range.

When inorganic solids and water are present, an electrolyte phase equilibrium model must be selected for the aqueous phase to properly account for the dissolution of the solid and formation of ions in solution.

4.3.4 User components

The process simulators were originally developed for petrochemical and fuels applications; consequently, many molecules that are made in specialty chemical and pharmaceutical processes are not listed in the component data banks. All of the simulators allow the designer to overcome this drawback by adding new molecules to customize the data bank.

In UniSim Design, new molecules are added as hypothetical components. The minimum information needed to create a new hypothetical pure component is the normal boiling point, although the user is encouraged to provide as much information as is available. If the boiling point is unknown, then the molecular weight and density are used instead. The input information is used to tune the UNIFAC correlation to predict the physical and phase equilibrium properties of the molecule, as described in Section 4.4.

User-defined components are created in Aspen Plus using a "user-defined component wizard." The minimum required information is the molecular weight and normal boiling point. The program also allows the designer to enter molecular structure, specific gravity, enthalpy and Gibbs energy of formation, ideal gas heat capacity, and Antoine vapor pressure coefficients, but for complex molecules usually only the molecular structure is known.

It is often necessary to add user components to complete a simulation model. The design engineer should always be cautious when interpreting simulation results for models that include user components. Phase equilibrium predictions for flashes, decanters, extraction, distillation, and crystallization operations should be carefully checked against laboratory data to ensure that the model is correctly predicting the component distribution between the phases. If the fit is poor, the binary interaction parameters in the phase equilibrium model can be tuned to improve the prediction.

4.4 Selection of physical property models

The process simulation programs all contain subroutines for calculating component and stream physical properties and for determining phase equilibrium in process operations. The user must select a thermodynamic model that provides a sufficiently accurate representation of the system for design purposes. When the design is sensitive to the choice of thermodynamic model, the models should be checked against measured data and the most accurate model selected. In some cases, it may be necessary to tune the library models in the simulator by adjusting some of the parameters to provide a better fit to the data.

4.4.1 Sources of physical property data

It is always a good practice to benchmark the physical properties predicted using a process simulation program against measured data. There are many good literature sources of data for properties of individual compounds, but much less data are available for mixtures. Caution should be exercised when taking data from the literature, as

typographical errors often occur. If a value looks suspicious, it should be cross-checked in an independent reference or by estimation.

The values of some properties are dependent on the method of measurement—for example, surface tension and flash point—and the method used should be checked by reference to the original paper, if necessary, if an accurate value is required.

International Critical Tables (ICT) (Washburn, 1933) is still probably the most comprehensive compilation of physical properties and is available in most reference libraries. Though it was first published in 1933, physical properties do not change, except in as much as experimental techniques improve, and ICT is still a useful source of engineering data. ICT is now available as an e-book and can be referenced on the Internet through Knovel (2003).

Tables and graphs of physical properties are given in many handbooks and textbooks on chemical engineering and related subjects. Many of the data given are duplicated from book to book, but the various handbooks do provide quick, easy access to data on the more commonly used substances.

An extensive compilation of thermophysical data has been published by Plenum Press (Touloukian, 1970−1977). This multiple-volume work covers conductivity, specific heat, thermal expansion, viscosity, and radiative properties (emittance, reflectance, absorptance, and transmittance).

The Engineering Sciences Data Unit (ESDU, www.ihsesdu.com) was set up to provide validated data for engineering design, developed under the guidance and approval of engineers from industry, the universities, and research laboratories. ESDU data include equipment design data and extensive high-quality physical property data—mostly for pure fluids that are in use in the oil and process industries.

The results of research work on physical properties are reported in the general engineering and scientific literature. The *Journal of Chemical Engineering Data* specializes in publishing physical property data for use in chemical engineering design. A quick search of the literature for data can be made by using the abstracting journals, such as *Chemical Abstracts* (American Chemical Society) and *Engineering Index* (Engineering Index, Inc.). *Engineering Index* is now called Engineering Information (Ei) and is a web-based reference source owned by Elsevier information (www.ei.org). *Chemical Abstracts* can be searched using the ACS SciFinder service.

Experimental phase equilibrium data have been published for several thousand binary and many multicomponent systems. Virtually all the published experimental data have been collected together in the volumes comprising the DECHEMA vapor−liquid and liquid−liquid data collection (DECHEMA, 1977). The books by Chu et al. (1956), Hala et al. (1968, 1973), Hirata et al. (1975), and Ohe (1989, 1990) are also useful sources.

Computerized physical property data banks have been set up by various organizations to provide a service to the design engineer. They can be incorporated into computer-aided design programs and are increasingly being used to provide reliable, authenticated design data. Examples of such programs are the Physical Property Data Service (PPDS) and the The Design Institue for Physical Properties (DIPPR) databases.

PPDS was originally developed in the United Kingdom by the Institution of Chemical Engineers and the National Physical Laboratory. It is now available as a Microsoft Windows version from NEL, a division of the TUV Suddeutschland Group (www.tuvnel.com/content/ppds.aspx). PPDS is made available to universities at a discount.

The DIPPR databases were developed by the Design Institute for Physical Properties of the AIChE. The DIPPR projects are aimed at providing evaluated process design data for the design of chemical processes and equipment (www.aiche.org/TechnicalSocieties/DIPPR/index.aspx). The DIPPR Project 801 has been made available to university departments; see Rowley et al. (2004).

Many of the important sources of engineering information are subscription services. The American Chemical Society's Chemical Abstracts Service is the best source for chemical properties and reaction kinetics data. Chemical abstracts can be searched online through the SciFinder subscription service (www.cas.org). This is available in most university libraries.

Another important source of information is Knovel. Knovel provides online access to most standard reference books. It is a subscription service but can be accessed through many libraries, including those of the professional engineering institutions and most universities. At the time of writing, Knovel is available for free to members of the AIChE. In addition to having many reference books in .pdf format, Knovel has interactive graphs and look-up tables for books such as *Perry's Chemical Engineers Handbook* and the *International Critical Tables.*

4.4.2 Prediction of physical properties

The process simulation programs contain subroutines that predict the physical properties of pure compounds and mixtures as functions of temperature, pressure, and composition. The algorithms used have been developed based on decades of research in thermodynamics and property estimation. Techniques are available for the prediction of

most physical properties, with sufficient accuracy for use in process and equipment design; however, the accuracy of the predictions should always be assessed by comparing the model output with data from experiments, pilot plants, or operating units. A detailed review of all the different methods available is beyond the scope of this book. If accurate values are required, then specialized texts on physical property estimation should be consulted, such as those by Reid et al. (1987), Poling et al. (2000), Bretsznajder (1971), Sterbacek et al. (1979), and AIChE (1983, 1985), and the data should be confirmed experimentally.

The techniques used for prediction are also useful for the correlation, and extrapolation and interpolation, of experimental values. The two most common approaches used in predicting properties are group contribution methods and the use of reduced properties.

Group contribution methods

Group contribution techniques are based on the concept that a particular physical property of a compound can be considered to be made up of contributions from the constituent atoms, groups, and bonds, with the contributions being determined from experimental data. They provide the designer with simple, convenient methods for physical property estimation, requiring only a knowledge of the structural formula of the compound.

Group contribution methods are used to predict a wide range of physical properties when no data are available for regression. For example, the group contribution method proposed by Chueh and Swanson (1973a, 1973b) gives reasonably accurate predictions of specific heat capacity for organic liquids. The contributions to be assigned to each molecular group are given in Table 4.2, and the method is illustrated in Example 4.1. The most widely used group contribution model is the UNIFAC method for predicting the parameters for phase equilibrium models.

TABLE 4.2 Group contributions for liquid heat capacities at 20 °C, kJ/kmol°C

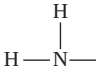
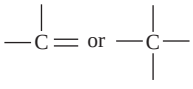
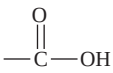
Group	Value	Group	Value
Alkane			
—CH_3	36.84		60.71
—CH_2—	30.40	—CH_2OH	73.27
	20.93		76.20
	7.37		111.37
Olefin		—OH	44.80
$=CH_2$	21.77	—ONO_2	119.32
	21.35	Halogen —Cl (first or second on a carbon) —Cl (third or fourth on a carbon)	36.01 25.12
	15.91	—Br	37.68
Alkyne		—F	16.75
—C≡H	24.70	—I	36.01
—C≡	24.70		
In a ring		Nitrogen	
	18.42		58.62
	12.14		43.96
—C=	22.19		31.40
—CH2—	25.96	—N=(in a ring)	18.84

TABLE 4.2 Group contributions for liquid heat capacities at 20 °C, kJ/kmol°C—cont'd

Group	Value	Group	Value
Oxygen		—C≡N	58.70
—O—	35.17	Sulphur	
	53.00	—SH	44.80
	53.00	—S—	33.49
		Hydrogen	
	79.97	H— (for formic acid, formates, hydrogen cyanide, etc.)	14.65

Add 18.84 for any carbon group that fulfils the following criterion: a carbon group that is joined by a single bond to a carbon group connected by a double or triple bond with a third carbon group. In some cases a carbon group fulfils this criterion in more ways than one; 18.84 should be added each time the group fulfils the criterion. Exceptions to the 18.84 rule:

1. *No such extra 18.84 additions for —CH_3 groups.*
2. *For a —CH_2— group fulfilling the 18.84 addition criterion, add 10.47 instead of 18.84. However, when the —CH_2— group fulfils the addition criterion in more ways than one, the addition should be 10.47 the first time and 18.84 for each subsequent addition.*
3. *No such extra addition for any carbon group in a ring.*

Source: Chueh and Swanson (1973a, 1973b).

Example 4.1

Using Chueh and Swanson's method, estimate the specific heat capacity of ethyl bromide at 20 °C.

Solution

Ethyl bromide CH_3CH_2Br

Group	Contribution	No. of	
—CH_3	36.84	1	= 36.84
—CH_2—	30.40	1	= 30.40
—Br	37.68	1	= 37.68
		Total	104.92 kJ/kmol°C

mol. wt. = 109

$$\text{Specific heat capacity} = \frac{104.92}{109} = \underline{\underline{0.96 \text{ kJ/kg°C}}}$$

Experimental value 0.90 kJ/kg°C

Reduced properties

Reduced property models (also known as *method of corresponding states models*) predict properties based on knowledge of the critical conditions of a compound. They are useful if values for the critical properties are available or can be estimated with sufficient accuracy; see Sterbacek et al. (1979). An example of a reduced property model is the method for estimating latent heat of vaporization developed by Haggenmacher (1946), which is derived from the Antoine vapor pressure equation:

$$L_v = \frac{8.32\, BT^2 \Delta z}{+(TC)^2} \tag{4.1}$$

where L_v = latent heat at the required temperature, kJ/kmol
T = temperature, K
B, C = coefficients in the Antoine equation (Antoine, 1888):

$$\ln P = A - \frac{B}{T + C} \tag{4.2}$$

where P = vapor pressure, mmHg
A, B, C = the Antoine coefficients
T = temperature, K

and
$\Delta z = z_{gas} - z_{liquid}$ (where z is the compressibility constant), calculated from the equation:

$$\Delta z = \left[1 - \frac{P_r}{T_r^3}\right]^{0.5} \tag{4.3}$$

P_r = reduced pressure = P/P_c
T_r = reduced temperature = T/T_c

Example 4.2

Estimate the latent heat of vaporization of acetic anhydride, $C_4H_6O_3$, at its boiling point, 139.6 °C (412.7 K) and at 200 °C (473 K).

Solution

For acetic anhydride $T_c = 569.1$ K, $P_c = 46$ bar

Antoine constants $A = 16.3982$
$B = 3287.56$
$C = -75.11$

Experimental value at the boiling point 41,242 kJ/kmol.
From the Haggenmacher equation:

$$\text{at the b.p. } P_r = \frac{1}{46} = 0.02124$$

$$T_r = \frac{412.7}{569.1} = 0.7252$$

$$\Delta z = \left[1 - \frac{0.02124}{0.7252^3}\right]^{0.5} = 0.972$$

$$L_{v,b} = \frac{8.32 \times 3287.6 \times (412.7)^2 \times 0.972}{(412.7 - 75.11)^2} = \underline{\underline{39,733 \text{kJ/mol}}}$$

At 200 °C, the vapor pressure must first be estimated from the Antoine equation:

$$\ln P = A - \frac{B}{T + C}$$

$$\ln P = 16.3982 - \frac{3287.56}{473 - 75.11} = 8.14$$

$$P = 3421.35 \text{ mmHg} = 4.5 \text{ bar}$$

$$P_r = \frac{4.5}{46} = 0.098$$

$$T_r = \frac{473}{569.1} = 0.831$$

$$\Delta z = \left[1 - \frac{0.098}{0.831^3}\right]^{0.5} = 0.911$$

$$L_v = \frac{8.32 \times 3287.6 \times (473)^2 \times 0.911}{(473 - 75.11)^2} = \underline{\underline{35,211 \text{ kJ/kmol}}}$$

If reliable experimental values of the critical constants cannot be found, techniques are available for estimating the critical constants with sufficient accuracy for most design purposes. For organic compounds Lydersen's method is normally used (Lydersen, 1955):

$$T_c = \frac{T_b}{\left[0.567 + \Sigma\Delta T - (\Sigma\Delta T)^2\right]} \tag{4.4}$$

$$P_c = \frac{M}{(0.34 + \Sigma\Delta P)^2} \tag{4.5}$$

$$V_c = 0.04 + \Sigma\Delta V \tag{4.6}$$

where T_c = critical temperature, K
P_c = critical pressure, atm (1.0133 bar)
V_c = molar volume at the critical conditions, m^3/kmol
T_b = normal boiling point, K
M = relative molecular mass
ΔT = critical temperature increments, Table 4.3
ΔP = critical pressure increments, Table 4.3
ΔV = molar volume increments, Table 4.3

TABLE 4.3 Critical constant increments

	ΔT	ΔP	ΔV		ΔT	ΔP	ΔV
Nonring increments							
—CH_3	0.020	0.227	0.055	$=\overset{\vert}{C}-$	0.0	0.198	0.036
$-\overset{\vert}{CH_2}$	0.020	0.227	0.055	$=C=$	0.0	0.198	0.036
$-\overset{\vert}{CH}\overset{\vert}{}$	0.012	0.210	0.051	$\equiv CH$	0.005	0.153	0.036*
$-\overset{\vert}{C}\overset{\vert}{}-$	0.00	0.210	0.041	$\equiv C-$	0.005	0.153	0.036*
$=CH_2$	0.018	0.198	0.045	H	0	0	0
$=\overset{\vert}{CH}$	0.018	0.198	0.045				
Ring increments							
—CH_2—	0.013	0.184	0.0445	$=\overset{\vert}{CH}$	0.011	0.154	0.037
$-\overset{\vert}{CH}\overset{\vert}{}$	0.012	0.192	0.046	$=\overset{\vert}{C}-$	0.011	0.154	0.036
$-\overset{\vert}{C}\overset{\vert}{}-$	−0.007*	0.154*	0.031*	$=C=$	0.011	0.154	0.036
Halogen increments							
—F	0.018	0.224	0.018	—Br	0.010	0.50*	0.070*
—Cl	0.017	0.320	0.049	—I	0.012	0.83*	0.095*

Continued

TABLE 4.3 Critical constant increments—cont'd

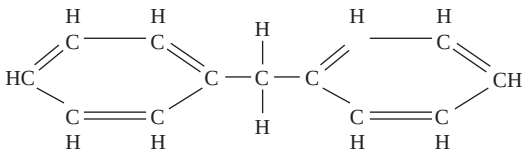
	ΔT	ΔP	ΔV		ΔT	ΔP	ΔV
Oxygen increments							
—OH (alcohols)	0.082	0.06	0.018*	—CO (ring)	0.033*	0.2*	0.050*
—OH (phenols)	0.031	−0.02*	0.030*	HC=O (aldehyde)	0.048	0.33	0.073
—O— (nonring)	0.021	0.16	0.020	—COOH (acid)	0.085	0.4*	0.080
—O— (ring)	0.014*	0.12*	0.080*	— COO— (ester)	0.047	0.47	0.080
—C=O (nonring)	0.040	0.29	0.060	==O (except for combinations noted earlier)	0.02*	0.12*	0.011*
Nitrogen increments							
$—NH_2$	0.031	0.095	0.028	—N— (ring)	0.007*	0.013*	0.032*
—NH (nonring)	0.031	0.135	0.037*	—CN	0.060*	0.36*	0.080*
—NH (ring)	0.024*	0.09*	0.027*	$—NO_2$	0.055*	0.42*	0.078*
—N— (nonring)	0.014	0.17	0.042*				
Sulfur increments							
—SH	0.015	0.27	0.055	—S— (ring)	0.008*	0.24*	0.045*
—S— (nonring)	0.015	0.27	0.055	S	0.003*	0.24*	0.047*
Miscellaneous							
—Si—	0.03	0.54*		—B—	0.03*		

Dashes represent bonds with atoms other than hydrogen.
Values marked with an asterisk are based on too few experimental points to be reliable.
Source: Lydersen (1955).

Lydersen's method illustrates how process simulation programs can predict the properties of user-specified components using just a molecular structure and a boiling point. Application of Lydersen's method generates critical constants, which can then be used in reduced parameter models to generate other properties. Although the final values that are predicted may still be suitable for preliminary design purposes, inaccuracy is introduced and propagated at each stage of such calculations, and the predictions should be confirmed against experimental values before detailed design.

Example 4.3

Estimate the critical constants for diphenylmethane using Lydersen's method: normal boiling point 537.5 K, molecular mass 168.2, structural formula:



Solution

Group	No. of	Total contribution ΔT	ΔP	ΔV
H—C(=)—(ring)	10	0.11	1.54	0.37
=C(—)—(ring)	2	0.022	0.308	0.072
—CH_2—	1	0.02	0.227	0.055
		Σ 0.152	2.075	0.497

$$T_c = \frac{537.5}{(0.567 + 0.152 - 0.152^2)} = \underline{\underline{772 \text{ k}}}$$

experimental value 767 K,

$$P_c = \frac{168.2}{(0.34 + 2.075)^2} = \underline{\underline{28.8 \text{ atm}}}$$

experimental value 28.2 atm,

$$V_c = 0.04 + 0.497 = \underline{\underline{0.537 \text{ m}^3/\text{kmol}}}$$

4.4.3 Phase equilibrium models

The choice of the best method for deducing vapor–liquid and liquid–liquid equilibria for a given system will depend on three factors:

1. The composition of the mixture (the system chemistry)
2. The operating pressure (low, medium, or high)
3. The experimental data available

The criterion for thermodynamic equilibrium between two phases of a multicomponent mixture is that for every component, i:

$$f_i^v = f_i^L \tag{4.7}$$

where f_i^v is the vapor phase fugacity and f_i^L the liquid phase fugacity of component i:

$$f_i^v = P\phi_i y_i \tag{4.8}$$

and

$$f_i^L = f_i^{OL}\gamma_i x_i \tag{4.9}$$

where P = total system pressure
ϕ_i = vapor fugacity coefficient
y_i = concentration of component i in the vapor phase
f_i^{OL} = standard-state fugacity of the pure liquid
γ_i = liquid phase activity coefficient
x_i = concentration of component i in the liquid phase

Substitution from Equations 4.8 and 4.9 into Equation 4.7 and rearranging gives:

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i f_i^{OL}}{P\varphi_i} \tag{4.10}$$

where K_i is the distribution coefficient (the K value)
ϕ_i can be calculated from an appropriate equation of state
f_i^{OL} can be computed from the following expression:

$$f_i^{OL} = P_i^o \phi_i^s \left\{ \exp\left[\frac{(P - P_i^o)}{RT} v_i^L \right] \right\} \tag{4.11}$$

where P_i^o = the pure component vapor pressure (which can be calculated from the Antoine equation, Equation 4.2), N/m^2

ϕ_i^s = the fugacity coefficient of the pure component i at saturation

v_i^L = the liquid molar volume, m^3/mol

The exponential term in Equation 4.11 is known as the *Poynting correction* and corrects for the effect of pressure on the liquid phase fugacity.

ϕ_i^s is calculated using the same equation of state used to calculate ϕ_i.

For systems in which the vapor phase imperfections are not significant, Equation 4.10 reduces to the familiar Raoult's law equation:

$$K_i = \frac{\gamma_i P_i^o}{P} \tag{4.12}$$

Vapor phase nonideality is usually modeled using an equation of state. An equation of state is a model for the molar volume of a real gas or liquid as a function of temperature and pressure. The features and limitations of the most commonly used equations of state are given in Table 4.4. For low-pressure systems with no known chemical interactions in the vapor phase, it is often acceptable to assume ideal gas behavior. For details of the equations, the reader should consult the reference cited or the books by Reid et al. (1987), Prausnitz et al. (1998), and Walas (1985). To select the best equation to use for a particular process design, refer to Fig. 4.2.

Liquid phase nonideality is encountered much more often than vapor phase nonideality and is modeled using activity coefficient models. The most frequently used activity coefficient models are the Wilson, NRTL, and UNIQUAC models summarized in Table 4.5. The simpler models that are taught in undergraduate thermodynamics classes are rarely adequate for design purposes.

TABLE 4.4 Equations of state

Model	Features	References
Redlich–Kwong Equation (R-K)	Redlich and Kwong (1949)	Extension of Van der Waal's equation, where constants are calculated from critical pressure and temperature. Not suitable for use near the critical pressure (P_r >0.8) or for liquids.
Redlich–Kwong–Soave Equation (R-K-S)	Soave (1972)	Modification to the R-K equation to extend its usefulness to the critical region and for use with liquids.
Benedict–Webb–Rubin Equation (B-W-R)	Benedict et al. (1951)	An eight-parameter empirical model that gives accurate predictions for vapor and liquid phase hydrocarbons. It can also be used for mixtures of light hydrocarbons with carbon dioxide and water.
Lee–Kesler–Plocker Equation (L-K-P)	Lee and Kesler (1975) Plocker et al. (1978)	Lee and Kesler extended the B-W-R equation to a wider variety of substances using the principle of corresponding states. The method was modified further by Plocker et al.
Chao–Seader Equation (C-S)	Chao and Seader (1961)	Gives accurate predictions for hydrogen and light hydrocarbons, but limited to temperatures below 530 K.
Grayson–Streed Equation (G-S)	Grayson and Streed (1963)	Extended the C-S equation for use with hydrogen-rich mixtures and for high-pressure and high-temperature systems. It can be used up to 200 bar and 4700 K.
Peng–Robinson Equation (P-R)	Peng and Robinson (1976)	Extension of the R-K-S equation to overcome instability in the R-K-S equation near the critical point.

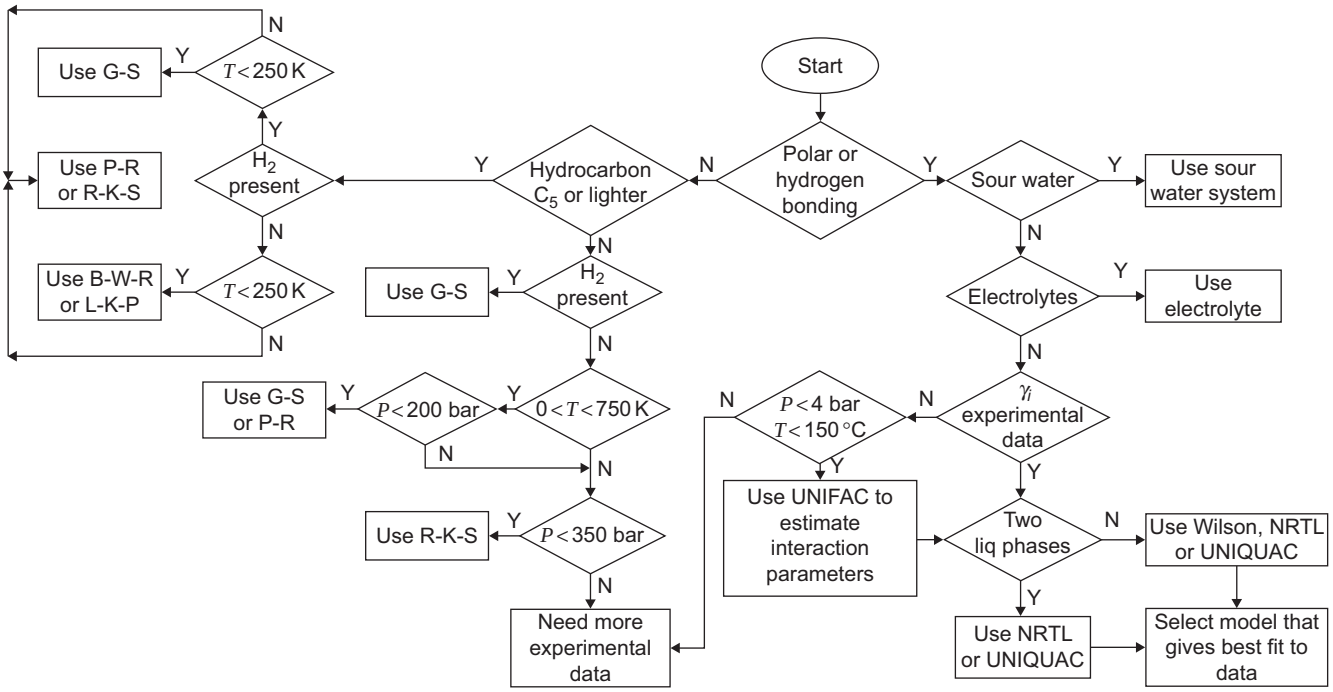


FIG. 4.2 Flow chart for the selection of phase equilibrium model.

TABLE 4.5 Activity coefficient models

Model	Features	References
Wilson Equation	Uses two adjustable parameters to model binary interactions between molecules. Can be extended to multicomponent systems using only binary parameters. Cannot predict formation of a second liquid phase.	Wilson (1964)
NRTL (Nonrandom Two-Liquid) Equation	Uses three parameters for each binary pair, where two are energies of interaction (similar to the Wilson parameters) and the third is a randomness factor that characterizes the tendency of molecules *i* and *j* to be distributed randomly in the mixture. Can predict liquid–liquid or vapor–liquid equilibrium.	Renon and Prausnitz (1969)
UNIQUAC (Universal Quasi-Chemical) Equation	Mathematically more complex than NRTL, but uses fewer adjustable parameters. Can predict liquid–liquid and vapor–liquid equilibrium. In the absence of experimental data, the parameters can be predicted by the UNIFAC method. Probably the most widely used model.	Abrams and Prausnitz (1975) Anderson and Prausnitz (1978a)

Activity coefficient models generally give good prediction of liquid phase fugacity for binary mixtures and can be extended to multicomponent mixtures if all the binary interaction parameters are known. The models become less reliable as the number of components increases, and the accuracy can be improved by fitting some data from ternary or higher-order mixtures.

The selection of the most appropriate liquid phase activity coefficient model for a given design is discussed in Section 4.4.5 and illustrated in Fig. 4.2.

The liquid phase activity coefficient, γ_i, is a function of pressure, temperature, and liquid composition. At conditions remote from the critical conditions, it is virtually independent of pressure and, in the range of temperature normally encountered in distillation, can be taken as independent of temperature. For a detailed discussion of the equations for activity coefficients and their relative merits, the reader is referred to the books by Reid et al. (1987), Prausnitz et al. (1998), Walas (1985), and Null (1970).

Most of the commercial process simulation programs contain subroutines that allow the user to enter phase-equilibrium data and perform a localized regression to better tune the binary interaction parameters in any of the

activity coefficient models. The binary interaction parameters are not unique constants, and locally adjusted parameters will provide more accurate prediction of phase equilibrium for a given design problem. Details of how to fit phase equilibrium data are given in the simulation program manuals.

4.4.4 Prediction of phase equilibrium constants

The designer will often be confronted with the problem of how to proceed with the design of a separation process without adequate experimentally determined equilibrium data. Some techniques are available for the prediction of vapor–liquid equilibrium (VLE) data and for the extrapolation of experimental values. The process simulation programs include libraries of measured data and interaction parameters for mixtures, as well as predictive methods. Caution must be used in the application of these techniques in design, and the predictions should be confirmed against experimentally determined values whenever practicable.

Group contribution methods

Group contribution methods have been developed for the prediction of liquid phase activity coefficients. The objective has been to enable the prediction of phase equilibrium data for the tens of thousands of possible mixtures of interest to the process designer to be made from the contributions of the relatively few functional groups that made up the compounds. The UNIFAC method—see Fredenslund, Gmehling, and Michelsen et al. (1977)—is probably the most useful for process design. Its use is described in detail in a book by Fredenslund, Gmehling, and Rasmussen et al. (1977). A method was also developed to predict the parameters required for the NRTL equation: the ASOG method—see Kojima and Tochigi (1979). More extensive work has been done to develop the UNIFAC method, to include a wider range of functional groups; see Gmehling et al. (1982) and Magnussen et al. (1981). The UNIFAC method can be used to estimate binary interaction parameters for the UNIQUAC model and, by extension, the NRTL and Wilson models.

Care must be exercised in applying the UNIFAC method. The specific limitations of the method are:

1. Pressure not greater than a few bar (say, limit to 5 bar)
2. Temperature below 150 °C
3. No noncondensable components or electrolytes
4. Components must not contain more than 10 functional groups

Sour water systems

The term *sour water* is used for water containing carbon dioxide, hydrogen sulfide, and ammonia encountered in refinery operations. Special correlations have been developed to handle the VLE of such systems, and these are incorporated in most design and simulation programs. Newman (1991) gives the equilibrium data required for the design of sour water systems as charts.

Electrolyte systems

When water and salts are present in a mixture, the salts can dissociate into ions in aqueous solution. The phase equilibrium model must account for dissociation and the presence of long-range interactions between charges on ions, as well as vapor–liquid or liquid–liquid equilibrium. Special electrolyte models and databases such as the OLI model have been developed for electrolyte systems. These models are available in the commercial process simulation programs, but sometimes require an additional fee.

Vapor–liquid equilibrium at high pressures

At pressures above a few atmospheres, the deviations from ideal behavior in the gas phase will be significant and must be taken into account in process design by use of a suitable equation of state for the vapor phase. The effect of pressure on the liquid phase activity coefficient must also be considered. A discussion of the methods used to correlate and estimate VLE data at high pressures is beyond the scope of this book. The reader should refer to the texts by Null (1970), Prausnitz et al. (1998), or Prausnitz and Chueh (1968).

Prausnitz and Chueh also discuss phase equilibrium in systems containing components above their critical temperature (supercritical components).

Liquid–liquid equilibrium

Experimental data, or predictions, that give the distribution of components between the two solvent phases are needed for the design of liquid–liquid extraction processes, and mutual solubility limits are needed for the design of decanters and other liquid–liquid separators.

Green and Perry (2007) give a useful summary of solubility data. Liquid–liquid equilibrium (LLE) compositions can be predicted from VLE data, but the predictions are rarely accurate enough for use in the design of liquid–liquid extraction processes. The DECHEMA data collection includes LLE data for several hundred mixtures (DECHEMA, 1977).

The UNIQUAC equation can be used to estimate activity coefficients and liquid compositions for multicomponent liquid–liquid systems. The UNIFAC method can be used to estimate UNIQUAC parameters when experimental data are not available. Some process simulation programs require the user to enable three-phase calculation or switch from a VLE mode to a VLLE mode when solving liquid–liquid equilibrium calculations.

It must be emphasized that extreme caution should be exercised when using predicted values for LLE in design calculations.

4.4.5 Choice of phase equilibrium model for design calculations

There is no universal algorithm for the selection of a phase equilibrium model. Although general rules can be given for the applicability of different equations of state, the models for liquid phase activity coefficients are semi-empirical, and it is often impossible to determine *a priori* which will provide the best fit to a set of experimental phase equilibrium data.

The flow chart shown in Fig. 4.2 has been adapted from a similar chart published by Wilcon and White (1986) and can be used as a preliminary guide to model selection. The abbreviations used in the chart for the equations of state and activity coefficient models correspond to those given in Tables 4.4 and 4.5. It must be emphasized that the best activity coefficient model is the model that provides the best fit to the experimental data over the range of interest. If no experimental data are available, then the best model is probably that for which the fewest interaction parameters must be estimated.

If a phase equilibrium model is created using estimated interaction parameters, the designer should highlight this as a source of uncertainty in the design. Before proceeding to detailed design, the design team should ensure that sufficient data are collected to confirm the model, and an expert on thermodynamics should be consulted to give advice on model selection and parameter estimation.

4.4.6 Validation of physical property models

The physical properties and phase equilibrium predicted by a process simulation program should always be validated by comparison with experimental measurements. It is not necessary to compare every parameter predicted by the model with real data, but any parameter that has a significant influence on the design should be confirmed. In some cases, it may also be necessary to confirm the accuracy of a physical property over a range of temperature or pressure.

In a revamp design, model validation is relatively straightforward, though usually not easy. A simulation model of the existing process can be built and tuned to match the current plant performance. Once the model is successfully benchmarked against the plant data, it can be used to evaluate new cases for the proposed design modifications. Although this sounds simple, the effort involved in matching a model to plant data can be considerable. It is often worthwhile to use a few independent laboratory experiments under more controlled conditions to reduce the number of parameters that are adjusted in the plant-based model.

Pilot plants and laboratory experiments can be a good source of data for model validation. When designing a pilot plant, consideration should be given to the need for collecting data to validate phase equilibrium models. Care must be taken to ensure that samples are taken when streams are at steady state and have had time to equilibrate.

If no experimental data are available, then it is usually a good idea to make an independent estimate of any parameters that have a strong influence on the design to be satisfied that the results from the simulator are credible. If the independent estimate does not agree with the simulation result, it may be worthwhile to conduct some experiments to collect real data. Methods for estimating physical properties are given in the book by Poling et al. (2000).

A flash calculation can be used as a simple technique for validating a phase equilibrium model when no data are available. The designer should set up a simulation model of a flash calculation using the temperature, pressure, and composition of interest. This simulation can then be run using different models for liquid and vapor phase nonideality that might be expected to be applicable to the system of interest. If the model predicts essentially the same stream flows and compositions regardless of the thermodynamic models selected, then the models are equally valid. This does not mean that the models are accurate, but at least they give the same results. If the flash calculation gives substantially different stream flows or compositions with different thermodynamic models, the designer should seek more experimental data with which to determine which model is most applicable.

4.5 Simulation of unit operations

A process simulation is built up from a set of unit operation models connected by mass and energy streams. The commercial simulators include many unit operation subroutines, sometimes referred to as *library models.* These operations can be selected from a palette or menu and then connected together using the simulator graphical user interface. Table 4.6 gives a list of the main unit operation models available in Aspen Plus and UniSim Design. Details of how to specify unit operations are given in the simulator manuals. This section provides general advice on unit operations modeling and modeling of nonstandard unit operations.

TABLE 4.6 Unit operation models in Aspen Plus and UniSim Design suites

Unit Operation	Aspen Plus Models	UniSim Design Models
Stream mixing	Mixer	Mixer
Component splitter	Sep, Sep2	Component Splitter
Decanter	Decanter	3-Phase Separator
Flash	Flash2, Flash3	Separator, 3-Phase Separator
Piping components		
Piping	Pipe, Pipeline	Pipe Segment, Compressible Gas Pipe
Valves & fittings	Valve	Valve, Tee, Relief Valve
Hydrocyclone	HyCyc	Hydrocyclone
Reactors		
Conversion reactor	RStoic	Conversion Reactor
Equilibrium reactor	REquil	Equilibrium Reactor
Gibbs reactor	RGibbs	Gibbs Reactor
Yield reactor	RYield	Yield Shift Reactor
CSTR	RCSTR	Continuous Stirred Tank Reactor
Plug flow reactor	RPlug	Plug Flow Reactor
Columns		
Shortcut distillation	DSTWU, Distl, SCFrac	Shortcut Column
Rigorous distillation	RadFrac, MultiFrac	Distillation, 3-Phase Distillation
Liquid-liquid extraction	Extract	Liquid-Liquid Extractor
Absorption and stripping	RadFrac	Absorber, Refluxed Absorber, Reboiled, Absorber
Fractionation	PetroFrac	3 Stripper Crude, 4 Stripper Crude, Vacuum Resid Column, FCCU Main, Fractionator

TABLE 4.6 Unit operation models in Aspen Plus and UniSim Design suites—cont'd

Unit Operation	Aspen Plus Models	UniSim Design Models
Rate-based distillation	RATEFRAC™	
Batch distillation	BatchFrac	
Heat transfer equipment		
Heater or cooler	Heater	Heater, Cooler
Heat exchanger	HeatX, HxFlux, Hetran, HTRI-Xist	Heat Exchanger
Air cooler	Aerotran	Air Cooler
Fired heater	Heater	Fired Heater
Multi-stream exchanger	MheatX	LNG Exchanger
Rotating equipment		
Compressor	Compr, MCompr	Compressor
Turbine	Compr, MCompr	Expander
Pump, hydraulic turbine	Pump	Pump
Solids handling		
Size reduction	Crusher	
Size selection	Screen	Screen
Crystallizer	Crystallizer	Crystallizer, Precipitation
Neutralization		Neutralizer
Solids washing	SWash	
Filter	Fabfl, CFuge, Filter	Rotary Vacuum Filter
Cyclone	HyCyc, Cyclone	Hydrocyclone, Cyclone
Solids decanting	CCD	Simple Solid Separator
Solids transport		Conveyor
Secondary recovery	ESP, Fabfl, VScrub	Baghouse Filter
User models	User, User2, User3	User Unit Op

4.5.1 Reactors

The modeling of real industrial reactors is usually the most difficult step in process simulation. It is usually easy to construct a model that gives a reasonable prediction of the yield of the main product, but the simulator library models are not sophisticated enough to fully capture all the details of hydraulics, mixing, mass transfer, catalyst and enzyme inhibition, cell metabolism, and other effects that often play a critical role in determining the reactor outlet composition, energy consumption, rate of catalyst deactivation, and other important design parameters.

In the early stages of process design, the simulator library models are usually used with simplistic reaction models that give the design engineer a good enough idea of yields and enthalpy changes to allow design of the rest of the process. If the design seems economically attractive, then more detailed models can be built and substituted into the flowsheet. These detailed models are usually built as user models, as described in Section 4.6 and Section 15.11.

Most of the commercial simulation programs have variants on the following reactor models.

Conversion reactor (stoichiometric reactor)

A conversion reactor requires a reaction stoichiometry and an extent of reaction, which is usually specified as an extent of conversion of a limiting reagent. No reaction kinetics information is needed, so it can be used when the

kinetics are unknown (which is often the case in the early stages of design) or when the reaction is known to proceed to full conversion. Conversion reactors can handle multiple reactions, but care is needed in specifying the order in which they are solved if they use the same limiting reagent.

Equilibrium reactor

An equilibrium reactor finds the equilibrium product distribution for a specified set of stoichiometric reactions. Phase equilibrium is also solved. The engineer can enter the outlet temperature and pressure and let the reactor model calculate the duty needed to reach that condition, or else enter a heat duty and let the model predict the outlet conditions from an energy balance.

An equilibrium reactor only solves the equations specified, so it is useful in situations where one or more reactions equilibrate rapidly while other reactions proceed much more slowly. An example is the steam reforming of methane to hydrogen. In this process, the water−gas shift reaction between water and carbon monoxide equilibrates rapidly at temperatures above 450 °C, whereas methane conversion requires catalysis even at temperatures above 800 °C. This process chemistry is explored in Example 4.5.

In some simulation programs, the equilibrium reactor model requires the designer to specify both liquid and vapor phase products, even though one of the streams may be calculated to have zero flow. If the real reactor has a single outlet, then the two product streams in the model should be mixed back together.

Gibbs reactor

The Gibbs reactor solves the full reaction and phase equilibrium of all species in the component list by minimization of the Gibbs free energy, subject to the constraint of the feed mass balance. A Gibbs reactor can be specified with restrictions such as a temperature approach to equilibrium or a fixed conversion of one species.

The Gibbs reactor is useful when modeling a system that is known to come to equilibrium, in particular, high-temperature processes involving simple molecules. It is less useful when complex molecules are present, as these usually have high Gibbs energy of formation; consequently, very low concentrations of these species are predicted unless the number of components in the model is highly restricted.

The designer must specify the components carefully when using a Gibbs reactor in the model, as the Gibbs reactor can only solve for specified components. If a component that is actually formed is not listed in the component set, then the Gibbs reactor results will be meaningless. Care must be taken to include all isomers, as the absence of isomers can distort the results of a Gibbs reactor. Furthermore, if some of the species have high Gibbs free energy, their concentrations may not be properly predicted by the model. An example is aromatic hydrocarbon compounds such as benzene, toluene, and xylenes, which have Gibbs free energy of formation greater than zero. If these species are in a model component set that also contains hydrogen and carbon, then a Gibbs reactor will predict that only carbon and hydrogen are formed. Although hydrogen and coke are indeed the final equilibrium products, the aromatic hydrocarbons are kinetically stable, and there are many processes that convert aromatic hydrocarbon compounds without significant coke yields. In this situation, the designer must either omit carbon from the component list or use an equilibrium reactor in the model.

Continuous stirred tank reactor

The continuous stirred tank reactor (CSTR) is a model of the conventional well-mixed reactor. It can be used when a model of the reaction kinetics is available and the reactor is believed to be well mixed (i.e., the conditions everywhere in the reactor are the same as the outlet conditions). By specifying forward and reverse reactions, the CSTR model can model equilibrium and rate-based reactions simultaneously. The main drawback of using the CSTR model is that a detailed understanding of kinetics is necessary if by-products are to be predicted properly.

Plug flow reactor

A plug flow reactor (PFR) models the conventional plug flow behavior, assuming radial mixing but no axial dispersion. The reaction kinetics must be specified, and the model has the same limitations as the CSTR model.

Most of the simulators allow heat input or removal from a PFR. Heat transfer can be with a constant wall temperature (as encountered in a fired tube, steam-jacketed pipe, or immersed coil) or with counter-current flow of a utility stream (as in a heat exchanger tube or jacketed pipe with cooling water).

Yield shift reactor

The yield shift reactor overcomes some of the drawbacks of the other reactor models by allowing the designer to specify a yield pattern. Yield shift reactors can be used when there is no model of the kinetics but some laboratory or pilot plant data are available, from which a yield correlation can be established.

Yield shift reactors are particularly useful when modeling streams that contain pseudocomponents, solids with a particle size distribution, or processes that form small amounts of many by-products. These can all be described easily in yield correlations, but can be difficult to model with the other reactor types.

The main difficulty in using the yield shift reactor is in establishing the yield correlation. If a single point—for example, from a patent—is all that is available, then entering the yield distribution is straightforward. If, on the other hand, the purpose is to optimize the reactor conditions, then a substantial set of data must be collected to build a model that accurately predicts yields over a wide enough range of conditions. If different catalysts can be used, the underlying reaction mechanism may be different for each, and each will require its own yield model. The development of yield models can be an expensive process and is usually not undertaken until corporate management has been satisfied that the process is likely to be economically attractive.

Modeling real reactors

Industrial reactors are usually more complex than the simple simulator library models. Real reactors usually involve multiple phases and have strong mass transfer, heat transfer, and mixing effects. The residence time distributions of real reactors can be determined by tracer studies and seldom exactly match the simple CSTR or PFR models; see Section 15.12.

Sometimes a combination of library models can be used to model the reaction system. For example, a conversion reactor can be used to establish the conversion of main feeds, followed by an equilibrium reactor that establishes an equilibrium distribution among specified products. Similarly, reactors with complex mixing patterns can be modeled as networks of CSTR and PFR models, as described in Sections 12.11.2 and 15.11.2 and illustrated in Fig. 12.14.

When using a combination of library models to simulate a reactor, it is a good idea to group these models in a sub-flowsheet. The sub-flowsheet can be given a suitable label, such as "reactor," that indicates that all the unit operations it contains are modeling a single piece of real equipment. This makes it less likely that someone else using the model will misinterpret it as containing additional distinct operations.

Detailed models of commercial reactors are usually written as user models. User models are described in Section 4.6. Detailed modeling of reactors is discussed in more detail in Section 15.11.

Example 4.4

When heavy oils are cracked in a catalytic or thermal cracking process, lighter hydrocarbon compounds are formed. Most cracking processes on heavy oil feeds form products with carbon numbers ranging from 2 to greater than 20. How does the equilibrium distribution of hydrocarbon compounds with five carbons (C_5 compounds) change as the temperature of the cracking process is increased at 200 kPa?

Solution

This problem was solved using UniSim Design.

The problem asks for an equilibrium distribution, so the model should contain either a Gibbs reactor or an equilibrium reactor.

A quick glance at the component list in UniSim Design shows that there are 22 hydrocarbon species with five carbons. To model the equilibrium among these species, we also need to include hydrogen to allow for the formation of alkenes, dienes, and alkynes. Although it would be possible to enter 21 reactions and use an equilibrium reactor, it is clearly easier to use a Gibbs reactor for this analysis. Fig. 4.3 shows the Gibbs reactor model.

To specify the feed we must enter the temperature, pressure, flow rate, and composition. The temperature, pressure, and flow rate are entered in the stream editor window (Fig. 4.4). The feed composition can be entered as 100% of any of the C_5 paraffin species, for example, normal pentane. The results from a Gibbs reactor would be the same if 100% isopentane was entered. It should be noted, however, that if a mixture of a pentane and a pentene were specified, then the overall ratio of hydrogen to carbon would be different and different results would be obtained.

A spreadsheet was also added to the model, as illustrated in Fig. 4.3, to make it easier to capture and download the results. The spreadsheet was set up to import component mole fractions from the simulation (Fig. 4.5). The simulation was then run for a range of temperatures, and after each run a new column was entered in the spreadsheet (Fig. 4.6).

When the results are examined, many of the individual species are present at relatively low concentrations. It thus makes sense to group some compounds together by molecular type, for example, adding all the dienes together and adding all the alkynes (acetylenes) together.

The spreadsheet results were corrected to give the distribution of C_5 compounds by dividing by one minus the mole fraction of hydrogen and then plotted to give the graph in Fig. 4.7.

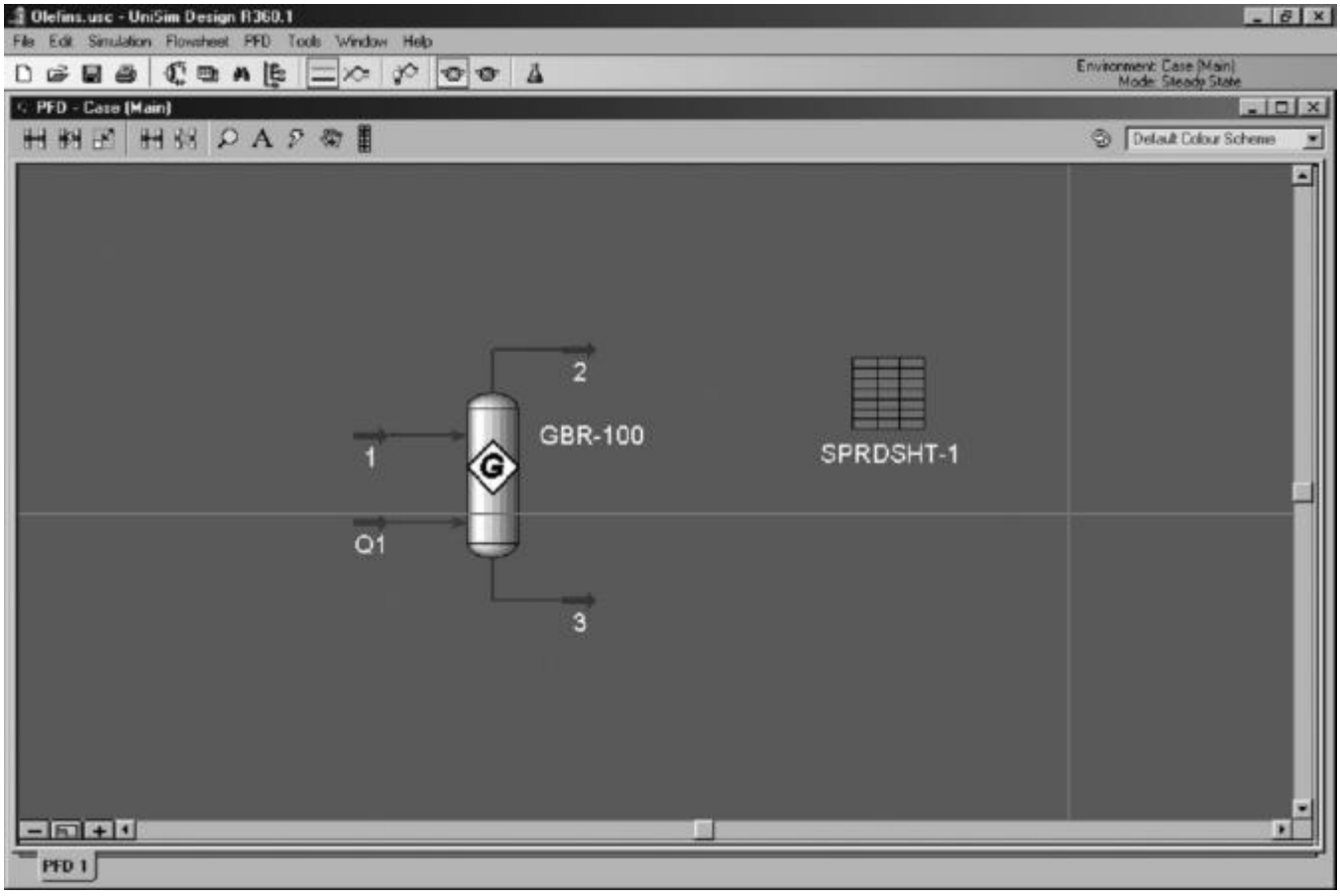


FIG. 4.3 Gibbs reactor model.

It can be seen from the graph that the equilibrium products at temperatures below 500 °C are mainly alkanes (also known as *paraffins* or *saturated hydrocarbons*), with the equilibrium giving roughly a 2:1 ratio of isopentane to normal pentane. As the temperature is increased from 500 °C to 600 °C, there is increased formation of alkene compounds (also known as *olefins*). At 700 °C, we see increased formation of cyclopentene and of dienes, and above 800 °C dienes are the favored product.

Of course this is an incomplete picture, as the relative fraction of C_5 compounds would be expected to decrease as the temperature is raised and C_5 species are cracked to lighter compounds in the C_2 and C_3 range. The model also did not contain carbon (coke) and so could not predict the temperature at which coke would become the preferred product. A more rigorous equilibrium model of a cracking process might include all of the possible hydrocarbon compounds up to C_7 or higher.

A real reactor might give a very different distribution of C_5 compounds from that calculated using the Gibbs reactor model. Dienes formed at high temperatures might recombine with hydrogen during cooling, giving a mixture that looked more like the equilibrium product at a lower temperature. There might also be formation of C_5 compounds by condensation reactions of C_2 and C_3 species during cooling, or loss of dienes and cyclopentene due to coke formation.

Example 4.5

Hydrogen can be made by steam reforming of methane, which is a highly endothermic process:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \qquad \Delta H^{\circ}_{rxn} = 2.1 \times 10^5 \text{ kJ/kgmol}$$

Steam reforming is usually carried out in fired tubular reactors, with catalyst packed inside the tubes and fuel fired on the outside of the tubes to provide the heat of reaction. The product gas mixture contains carbon dioxide and water vapor, as well as carbon monoxide and hydrogen, and is conventionally known as *synthesis gas* or *syngas*.

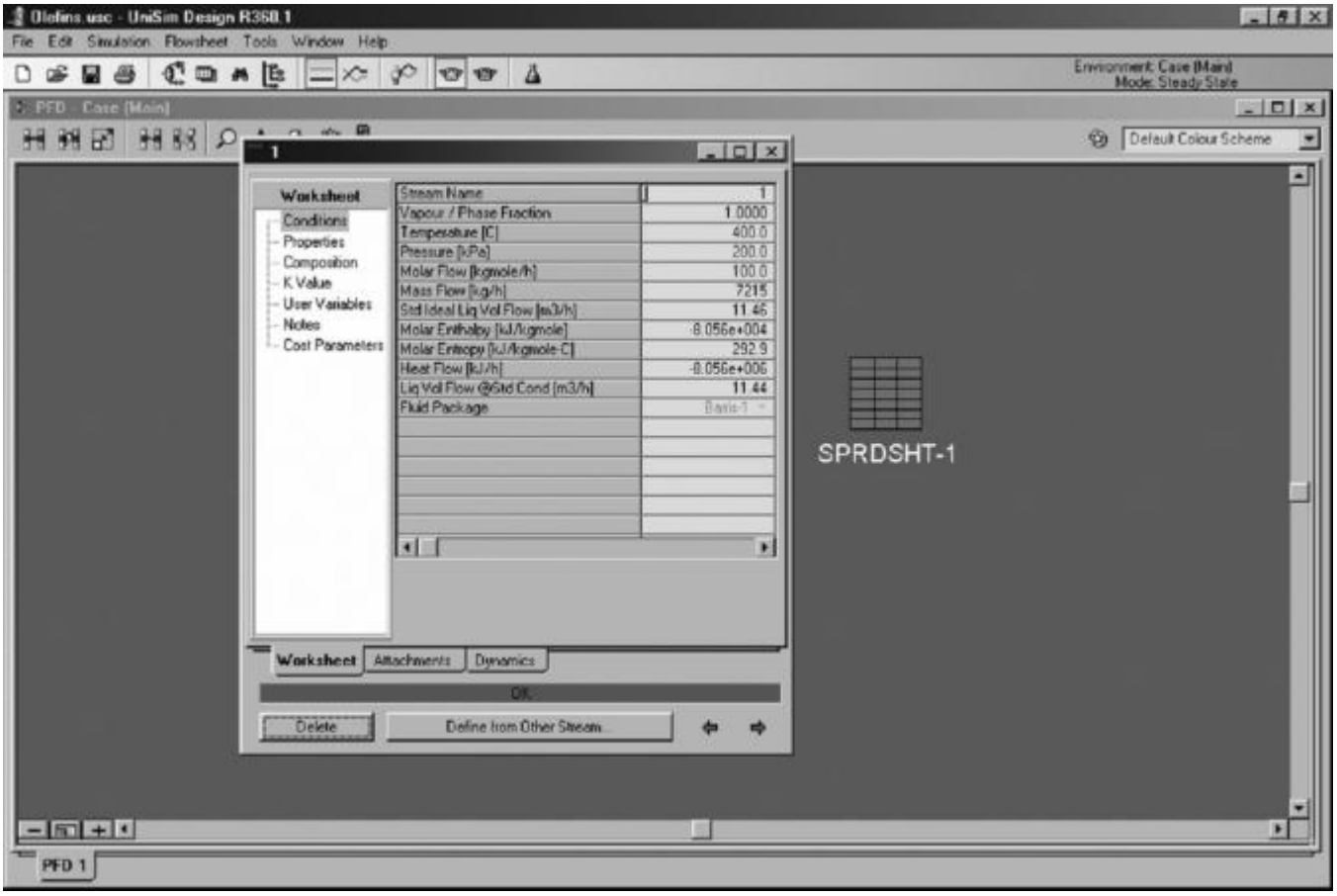


FIG. 4.4 Stream entry.

Hydrogen can also be made by partial oxidation of methane, which is an exothermic process, but yields less product per mole of methane feed:

$$CH_4 + \tfrac{1}{2}O_2 \rightarrow CO + 2H_2 \qquad \Delta H^{\circ}_{rxn} = -7.1 \times 10^4 \text{ kJ/kgmol}$$

When steam, oxygen, and methane are combined, heat from the partial oxidation reaction can be used to provide the heat for steam reforming. The combined process is known as *autothermal reforming*. Autothermal reforming has the attraction of requiring less capital investment than steam reforming (because it does not need a fired-heater reactor), but giving higher yields than partial oxidation.

The yield of hydrogen can be further increased by carrying out the water–gas shift reaction:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \Delta H^{\circ}_{rxn} = -4.2 \times 10^4 \text{ kJ/kgmol}$$

The water–gas shift reaction equilibrates rapidly at temperatures above about 450 °C. At high temperatures this reaction favors the formation of carbon monoxide, whereas at low temperatures more hydrogen is formed. When hydrogen is the desired product, the shift reaction is promoted at lower temperatures by using an excess of steam and providing a medium- or low-temperature shift catalyst.

In an autothermal reforming process, 1000 kmol/h of methane at 20 °C is compressed to 10 bar, mixed with 2500 kmol/h of saturated steam, and reacted with pure oxygen to give 98% conversion of the methane. The resulting products are cooled and passed over a medium-temperature shift catalyst that gives an outlet composition corresponding to equilibrium at 350 °C.

1. How much heat is required to vaporize the steam?
2. How much oxygen is needed?
3. What is the temperature at the exit of the autothermal reforming reactor?
4. What is the final molar flow rate of each component of the synthesis gas?

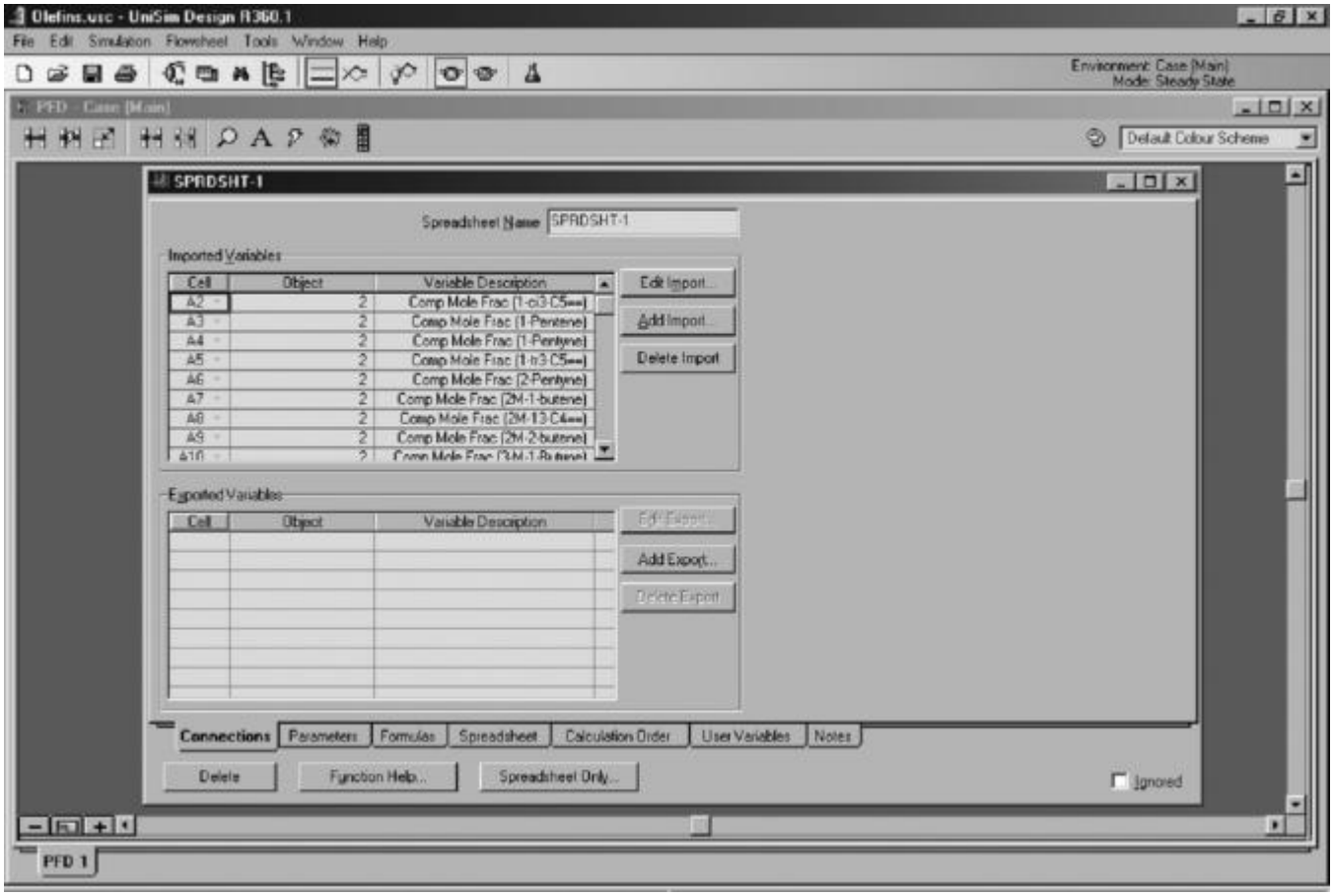


FIG. 4.5 Product composition spreadsheet.

Solution

This problem was solved using Aspen Plus. The model must simulate the high-temperature reforming reaction and the re-equilibration of the water–gas shift reaction as the product gas is cooled. A Gibbs reactor can be used for the high-temperature reaction, but an equilibrium reactor must be specified for the shift reactor, as only the water–gas shift reaction will re-equilibrate at 350 °C. Because the methane compressor supplies some heat to the feed, it should be included in the model. Because the question asks how much heat is needed to vaporize the steam, a steam boiler should also be included. The oxygen supply system can also be included, giving the model shown in Fig. 4.8.

The heat duty to the reforming reactor is specified as zero. The oxygen flow rate can then be adjusted until the desired methane conversion is achieved. For 98% conversion, the flow rate of methane in the autothermal reactor product (stream 502) is 2% of the flow rate in the reactor feed (stream 501) (i.e., 20 kmol/h). For the purpose of this example, the oxygen flow rate was adjusted manually, although a controller could have been used, as described in Section 4.8. The results are shown in Fig. 4.9.

When the simulation model was run, the following values were calculated:

1. The steam heater requires 36MW of heat input.
2. 674 kmol/h of oxygen are needed.
3. The temperature at the exit of the reforming reactor is 893 °C.
4. The molar flow rates at the outlet of the shift reactor (stream 504) are:

H_2	2504
H_2O	1956
CO	68
CO_2	912
CH_4	20

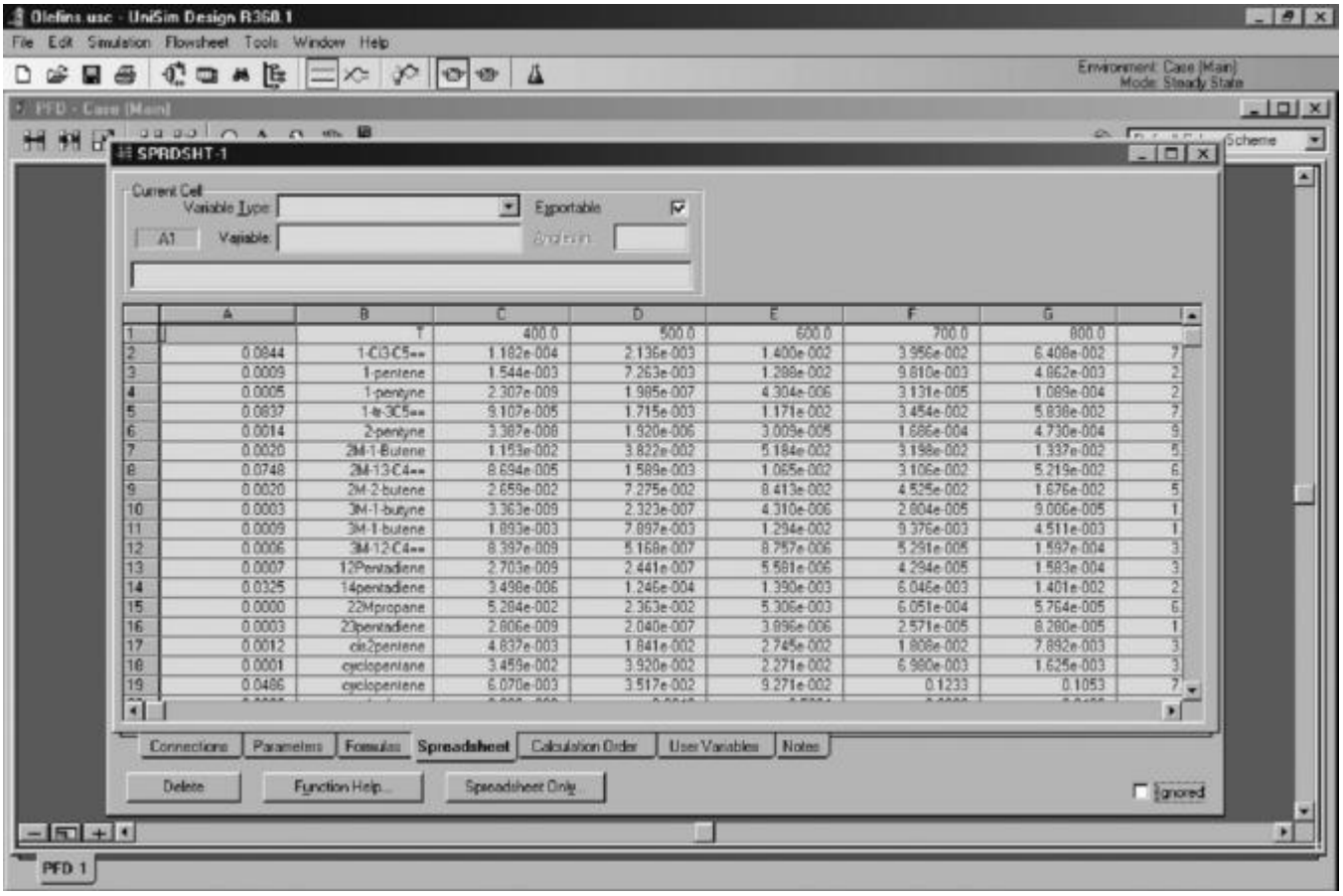


FIG. 4.6 Spreadsheet results.

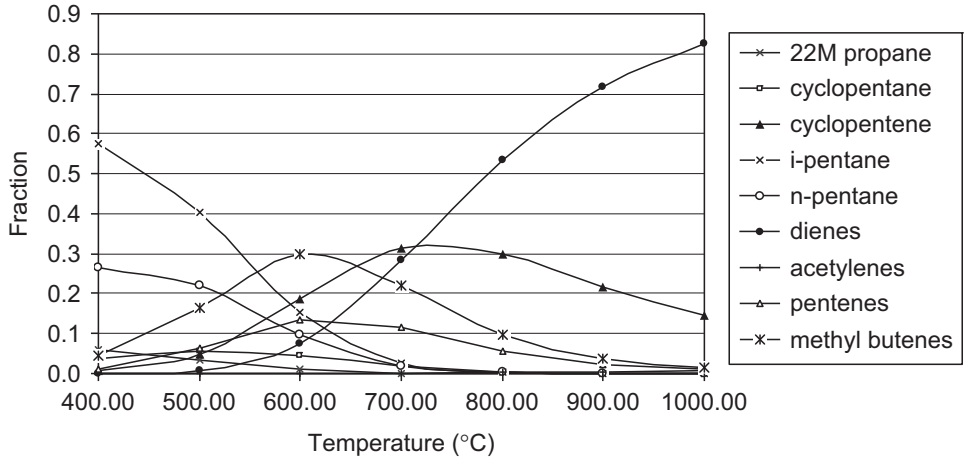


FIG. 4.7 Product distribution.

It should be immediately apparent from the model output that the process as simulated is far from optimal. The oxygen consumption is larger than the 500 kmol/h that would have been needed for partial oxidation. The excess oxygen is needed because the additional steam that is being fed must also be heated to the reactor outlet temperature, which requires more of the feed methane to be burned. The corollary of this result is that the hydrogen yield, at roughly 2.5 moles per mole methane, is not much better than could have been obtained with partial oxidation followed by shift, despite the large excess of steam used.

The designer has several options that could be examined to improve this process:

1. Increase heat recovery from the product gas to the feed streams to pre-heat the reactor feed and reduce the amount of oxygen that is needed.
2. Reduce the amount of steam fed with the methane.

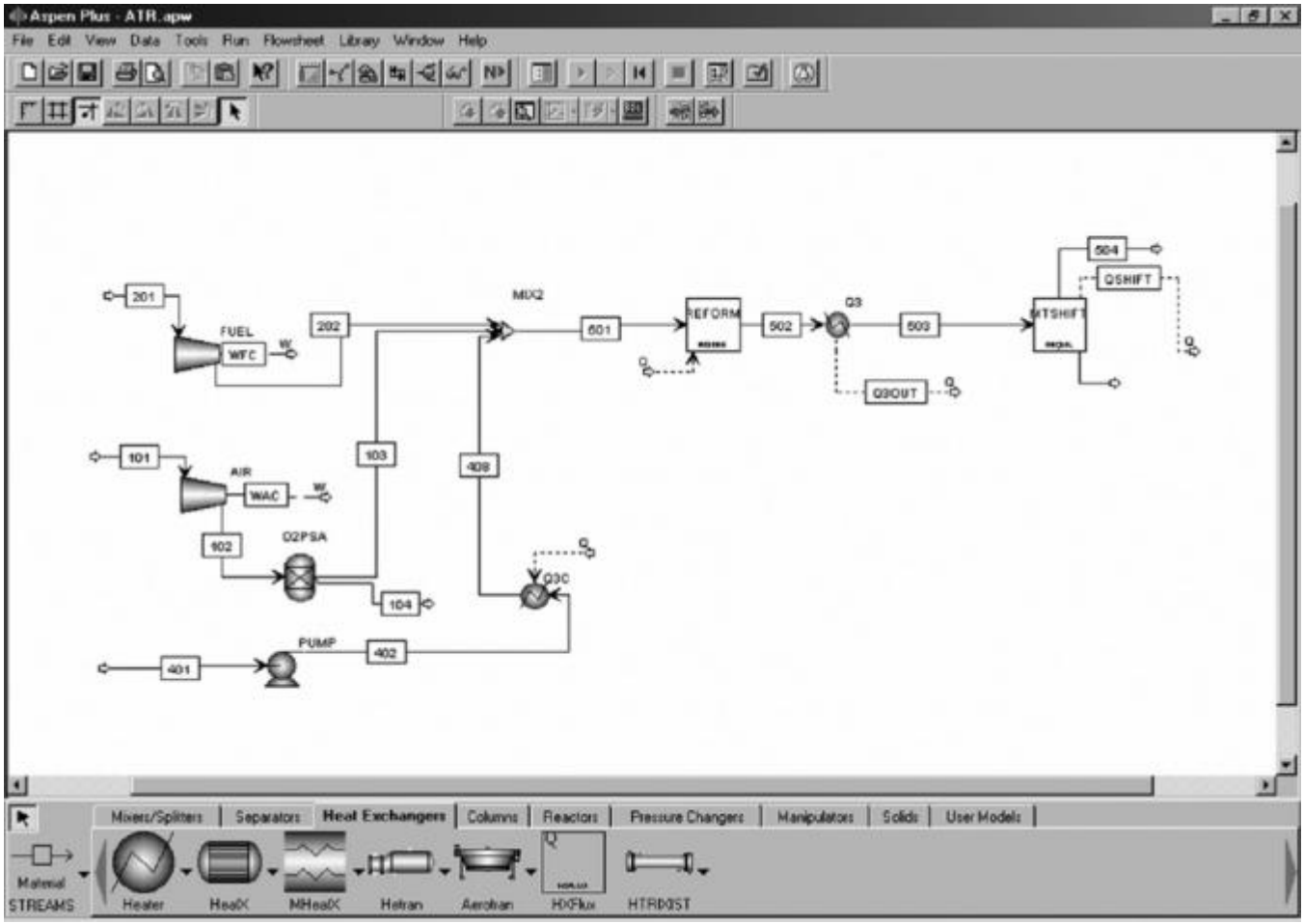


FIG. 4.8 Authothermal reforming model.

3. Bypass a part of the steam from the reformer feed to the shift reactor feed so as to obtain the benefit of driving the equilibrium in the shift reactor without the cost of providing extra heat to the reformer.
4. Reduce the conversion of methane so that a lower reactor conversion and lower outlet temperature are required.

In practice, all of these options are implemented to some extent to arrive at the optimal autothermal reforming conditions. This optimization is explored further in Problem 4.13.

4.5.2 Distillation

The commercial process simulators contain a range of distillation models with different degrees of sophistication. The design engineer must choose a model that is suitable for the purpose, depending on the problem type, the extent of design information available, and the level of detail required in the solution. In some cases, it may make sense to build different versions of the flowsheet, using different levels of detail in the distillation models, so that the simpler model can be used to initialize a more detailed model.

Shortcut models

The simplest distillation models to set up are the shortcut models. These models use the Fenske–Underwood–Gilliland or Winn–Underwood–Gilliland method to determine the minimum reflux and number of stages, or to determine the required reflux given a number of trays, or to determine the required number of trays for a given reflux ratio. These methods are described in Chapter 17. The shortcut models can also estimate the condenser and reboiler duties and determine the optimum feed tray.

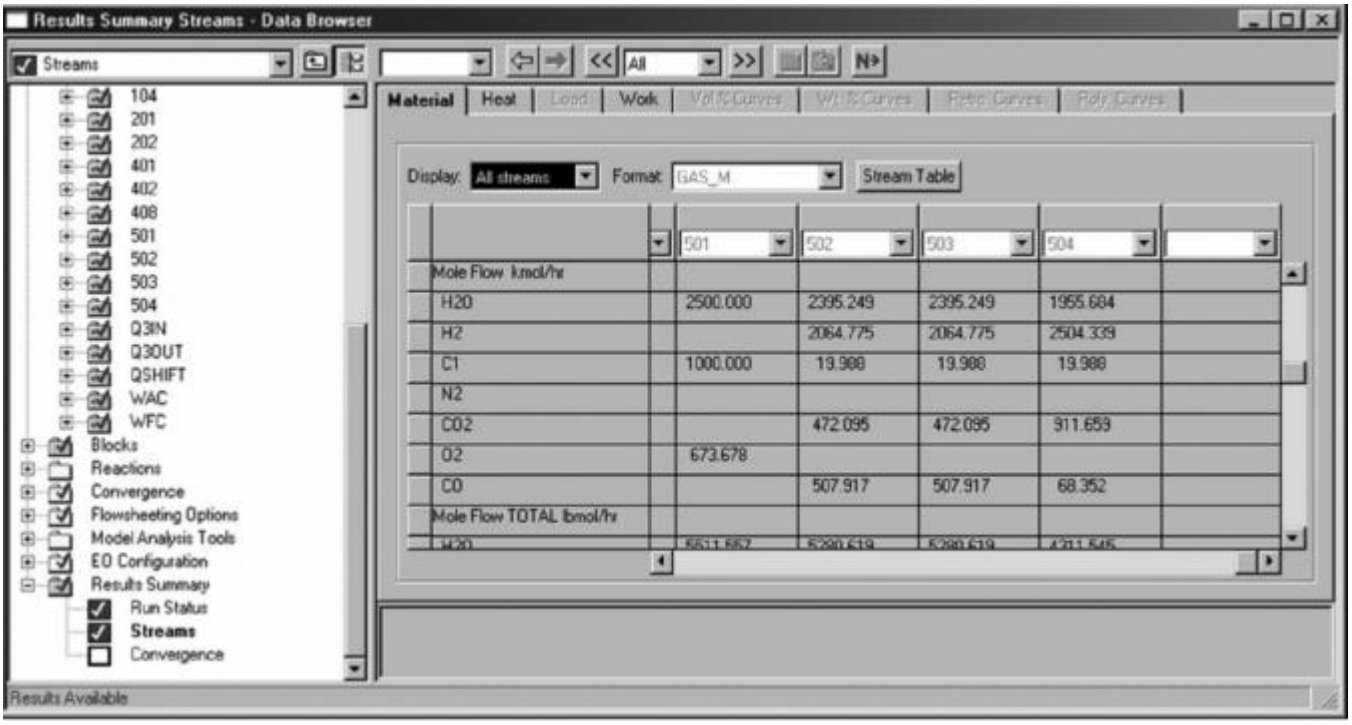


FIG. 4.9 Autothermal reactor model results.

The minimum information needed to specify a shortcut distillation model is:

- The component recoveries of the light and heavy key components
- The condenser and reboiler pressures
- Whether the column has a total or partial condenser

In some cases, the designer can specify the purities of the light and heavy key components in the bottoms and distillate, respectively. Care is needed when using purity as a specification, as it is easy to specify purities or combinations of purity and recovery that are infeasible.

The easiest way to use a shortcut distillation model is to start by estimating the minimum reflux and number of stages. The optimum reflux ratio is usually between 1.05 and 1.25 times the minimum reflux ratio, R_{min}, so $1.15 \times R_{min}$ is often used as an initial estimate. Once the reflux ratio is specified, the number of stages and optimum feed stage can be determined. The shortcut model results can then be used to set up and initialize a rigorous distillation simulation.

Shortcut models can also be used to initialize fractionation columns (complex distillation columns with multiple products), as described next.

Shortcut distillation models are robust and are solved quickly. They do not give an accurate prediction of the distribution of nonkey components, and they do not perform well when there is significant liquid phase nonideality, but they are an efficient way of generating a good initial design for a rigorous distillation model. In processes that have a large number of recycle streams, it is often worthwhile to build one model with shortcut columns and a second model with rigorous columns. The simple model will converge more easily and can be used to provide good initial estimates of column conditions and recycle streams for the detailed model.

The main drawback of shortcut models is that they assume constant relative volatility, usually calculated at the feed condition. If there is significant liquid or vapor phase nonideality, constant relative volatility is a very poor assumption, and shortcut models should not be used.

Rigorous models

Rigorous models carry out full stage-by-stage mass and energy balances. They give better predictions of the distribution of components than shortcut models, particularly when the liquid phase behaves nonideally, as the flash

calculation is made on each stage. Rigorous models allow many more column configurations, including use of side streams, intermediate condensers and reboilers, multiple feeds and side strippers and rectifiers. Rigorous models can be much harder to converge, particularly if poor initial estimates are used or if the column is improperly specified.

The two main types of rigorous distillation models are equilibrium-stage models and rate-based models. Equilibrium-stage models assume either full VLE on each stage or else an approach to equilibrium based on a stage efficiency entered by the designer. When using an equilibrium-stage model for column sizing, the stage efficiencies must be entered. Stage efficiency is typically less than 0.8 and is discussed in more detail in Chapter 17. Rate-based models do not assume phase equilibrium, except at the VLE, and instead solve the interphase mass transfer and heat transfer equations. Rate-based models are more realistic than the idealized equilibrium-stage models, but because it can be difficult to predict the interfacial area and mass transfer coefficients, rate-based models are less widely used in practice.

Rigorous distillation models can be used to model absorber columns, stripper columns, refluxed absorbers, three-phase systems such as extractive distillation columns, many possible complex column configurations, and columns that include reactions such as reactive distillation and reactive absorption columns. The formation of a second liquid phase (usually a water phase) in the column can be predicted if the designer has selected a liquid phase activity model that allows for the prediction of two liquid phases.

One of the most useful features of the rigorous distillation models in the commercial simulation programs is that most include a tool for plotting column profiles. The design engineer can generate plots showing the molar composition of each species in either phase versus tray number. These plots can be helpful in troubleshooting column designs.

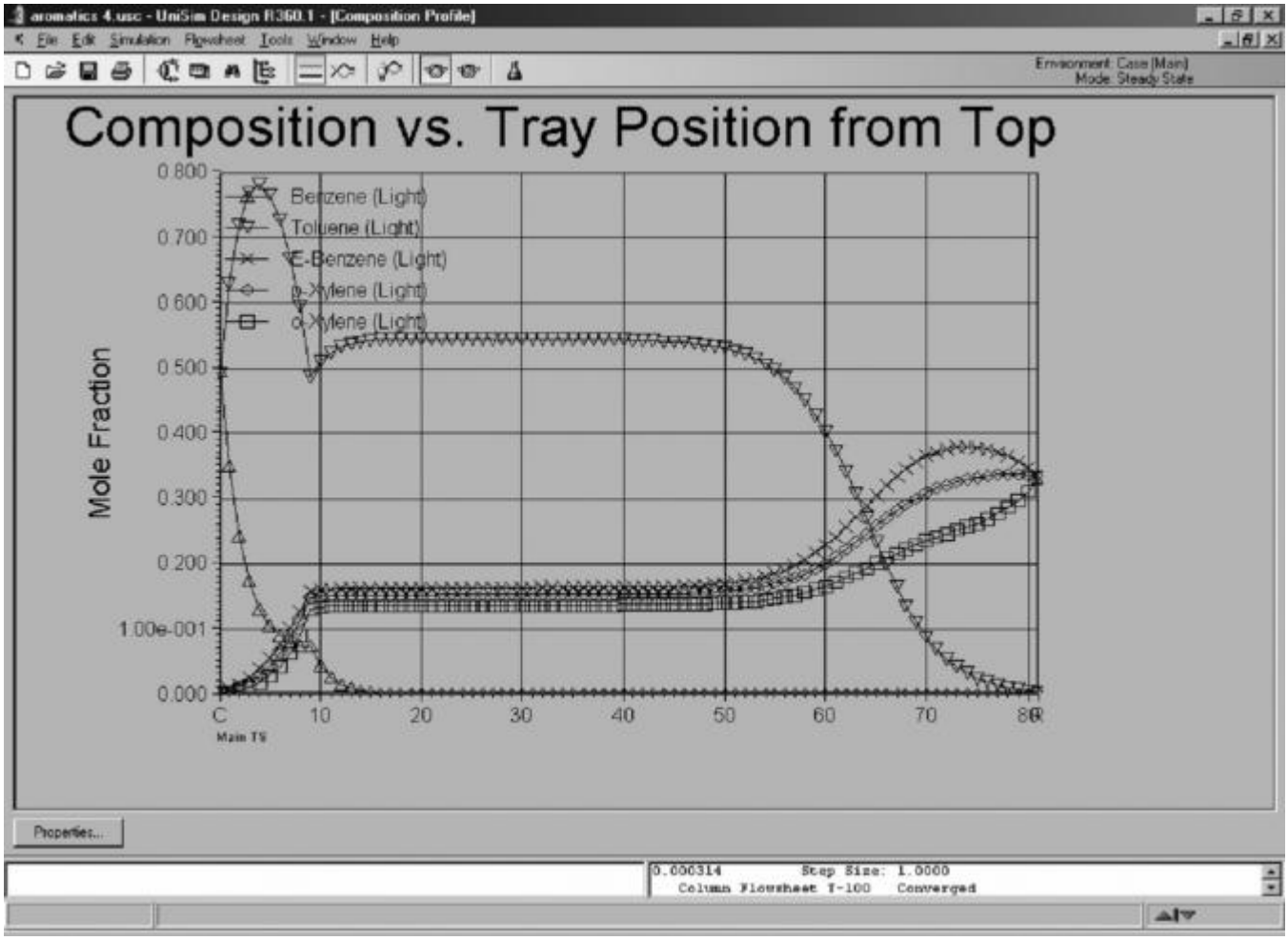


FIG. 4.10 Feed tray too high.

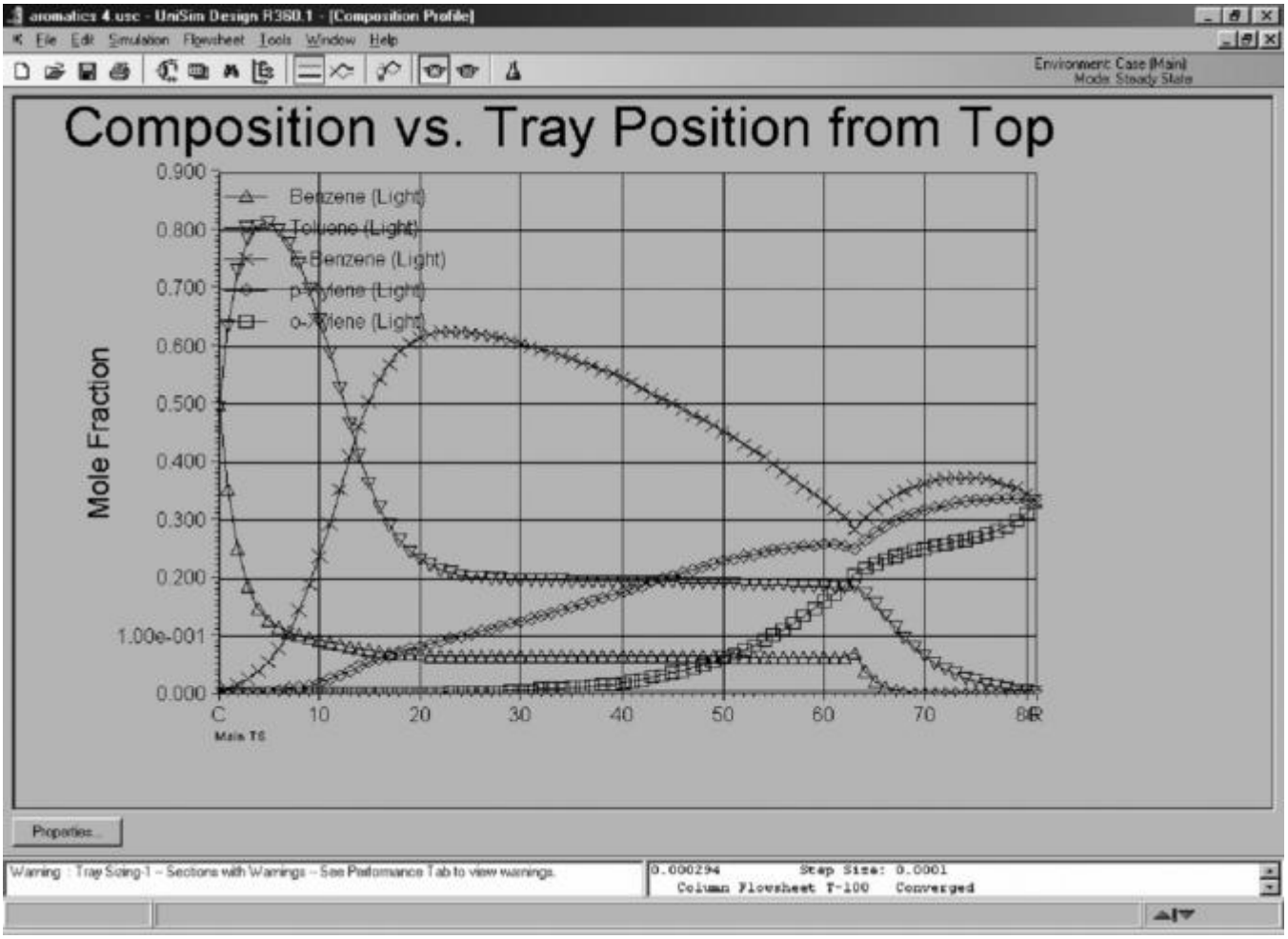


FIG. 4.11 Feed tray too low.

For example, Figs. 4.10 to 4.15 show column profiles for the distillation problem introduced in Examples 4.6 and 4.7, which is optimized in Example 12.1. The column was simulated in UniSim Design.

- In Fig. 4.10, the feed stage was moved up to tray 10, which is too high. The column profiles show a broad flat region between trays 20 and 45, indicating that nothing much is going on over this part of the column. There are too many trays in the stripping section, and the feed tray should be moved lower. Sections with very small change in composition can also be indicative of pinched regions where an azeotropic mixture is being formed.
- In Fig. 4.11, the feed tray has been moved down to tray 63, which is too low. The column profiles for benzene and toluene, the light components, are flat between trays 30 and 60 in the rectifying section, indicating that the feed tray should be moved higher.
- In Fig. 4.12, the column specification was changed from toluene recovery to reflux ratio, and a low value of reflux ratio (2.2) was entered. This is less than the minimum reflux required for the specified separation; consequently, the desired recovery of toluene cannot be achieved. The recovery of toluene is reduced to 72%.
- In Fig. 4.13, the reflux ratio was increased to 4.0. The recovery of toluene is now 100%, which is greater than the 99% required. This represents a suboptimal use of energy and capital.
- Fig. 4.14 shows the column profiles when the number of trays was reduced to 25, with the feed on tray 8. The column profile for toluene shows that there are insufficient stages (and/or reflux). Although the profile is changing smoothly, the recovery in the distillate is only 24.5%.
- The column profiles with the optimum conditions determined in Example 12.1 are shown in Fig. 4.15. The poor features shown in the other profiles are absent.

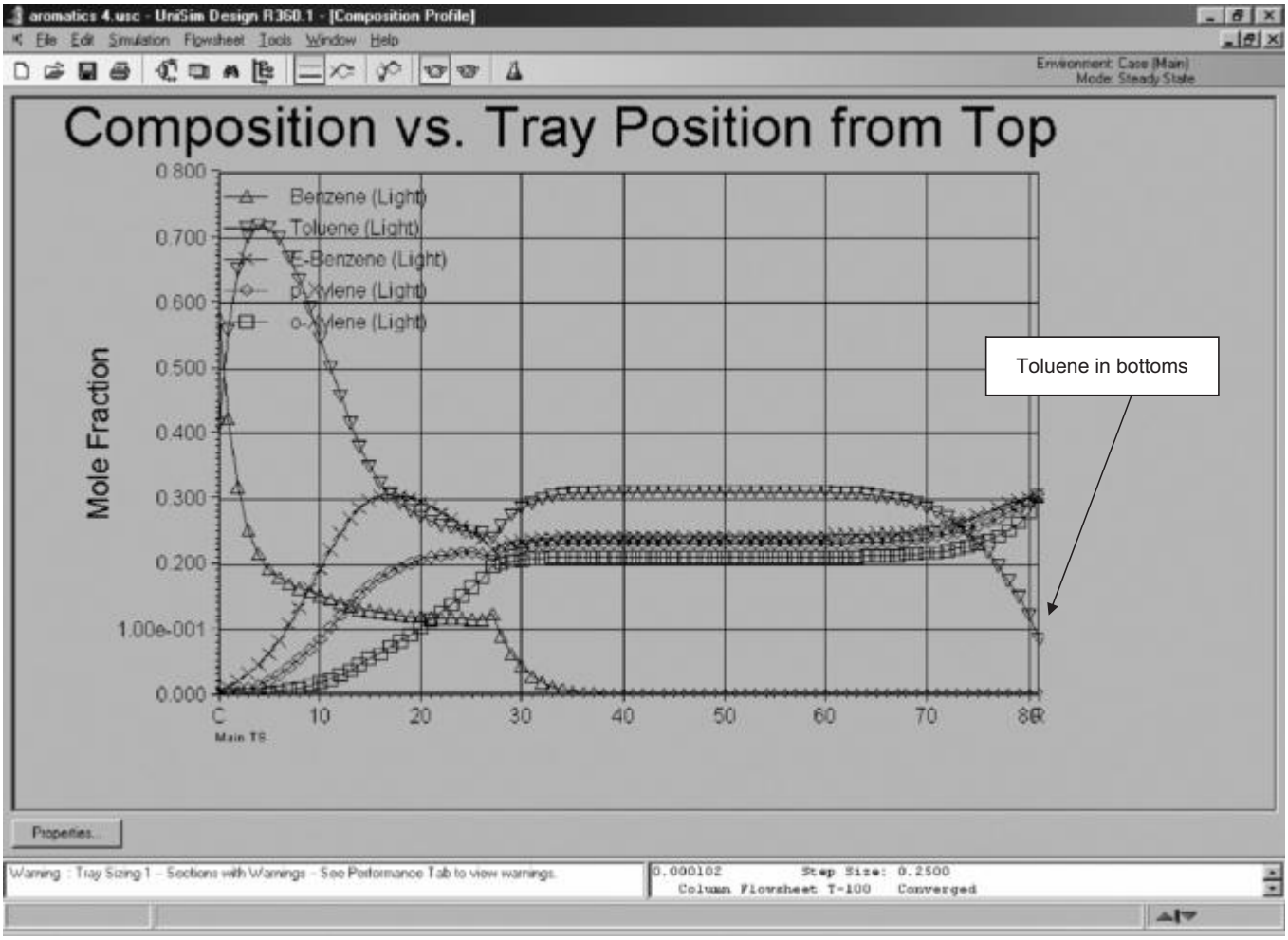


FIG. 4.12 Reflux ratio too low: Toluene recovery 72%.

Column convergence

Convergence of distillation column models is probably the most common problem in process simulation for novice engineers. There are many reasons why rigorous distillation models (and models of other multistage operations) may fail to converge. The most common causes of convergence problems are as follows:

- **Infeasible specifications:** In multicomponent distillation, care must be taken when using purity as a specification. It will not be possible to make a 99% pure distillate if the feed contains 2% of a component that boils lighter than the light key. The choice of column specifications is discussed in more detail in Section 17.6.2.
- **Poor initialization:** If the simulation model is set up with fewer than the minimum number of trays or less than the minimum reflux, it will not converge. Shortcut models can be used to provide an initial design that is feasible, which can then be used as a starting point for a rigorous model.
- **Poor initial estimates**: The faster distillation column solution algorithms (such as the widely used inside-out algorithm, discussed in Section 17.8.2) run much better when provided with a good initial estimate of tray temperatures.

A good practice is to start by using simple hand calculations to check that the column specifications are feasible. A shortcut model can then be used to determine the minimum reflux and the number of trays and feed tray location when the reflux is increased to about 1.1 times minimum reflux. The rigorous model should then be initialized with the reboiler and condenser temperatures found from the shortcut simulation, a linear temperature profile, and a pressure gradient that makes an approximate allowance for the pressure drop per tray (about 2 inches of liquid is typical).

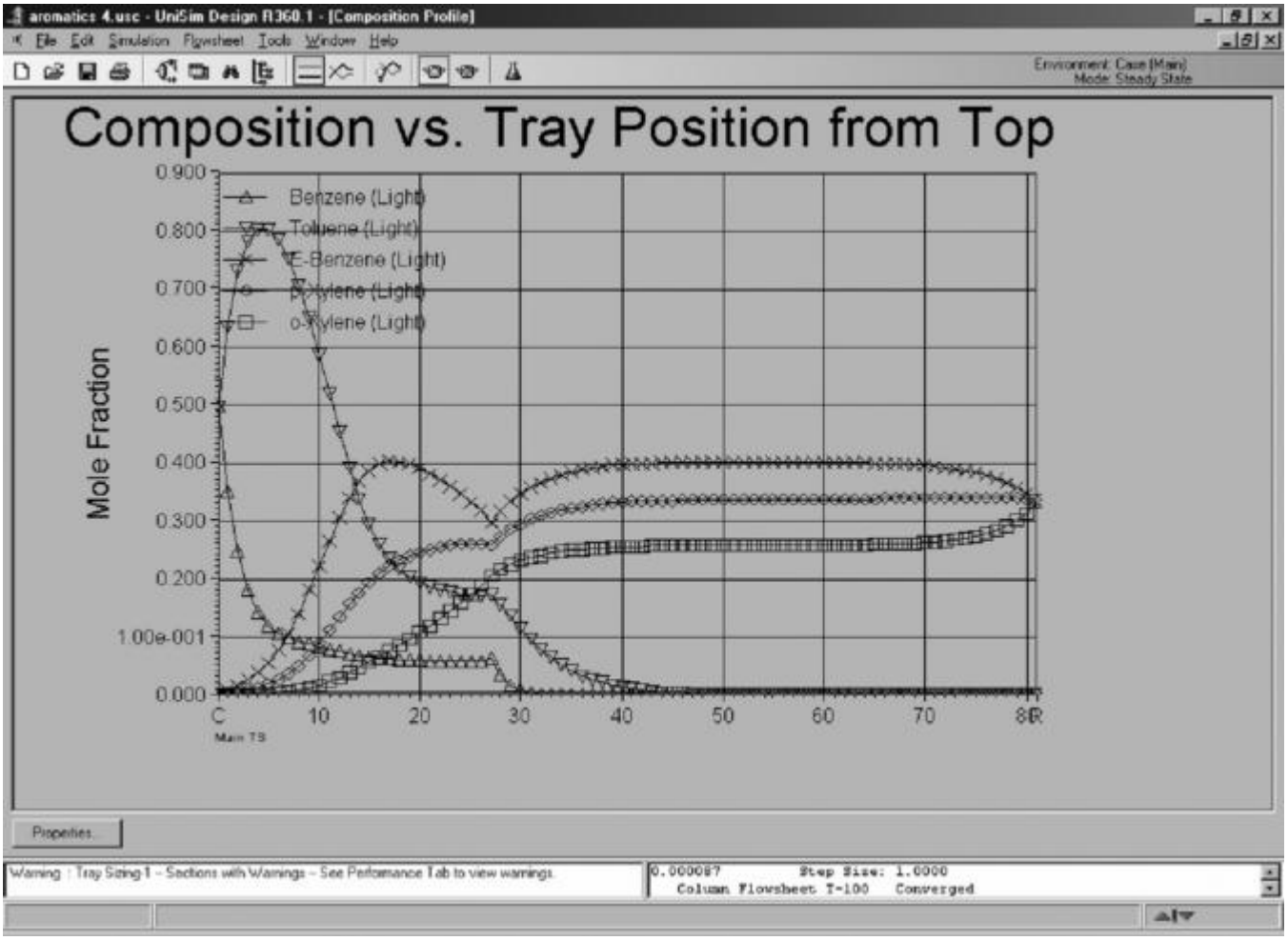


FIG. 4.13 Reflux ratio too high: Toluene recovery 100%.

If the inside-out algorithm is used, the rigorous model should initially be run with easy specifications, such as reflux ratio and either distillate rate or bottoms rate. These will guarantee convergence and generate a realistic column temperature profile that can then be stored as the estimate for future runs. The model specifications can then be changed to the desired design specifications (purity or recovery specifications), and now that the model has a good initialization and set of estimates, convergence will usually be rapid.

In the event that this method fails to give quick convergence, the designer should check that the specifications are feasible, check for existence of azeotropes, try adding trays, and examine the column profiles for clues to the problem.

Complex columns for fractionation

Several of the commercial simulation programs offer preconfigured complex column rigorous models for petroleum fractionation. These models include charge heaters, several side strippers, and one or two pump-around loops. These fractionation column models can be used to model refinery distillation operations such as crude oil distillation, vacuum distillation of atmospheric residue oil, fluidized catalytic cracking (FCC) process main columns, and hydrocracker or coker main columns. Aspen Plus also has a shortcut fractionation model, SCFrac, which can be used to configure fractionation columns in the same way that shortcut distillation models are used to initialize multicomponent rigorous distillation models.

A typical crude oil distillation column is illustrated in Fig. 4.16, which shows a simulation using an Aspen Plus PetroFrac model. The crude oil is pre-heated in a heat-exchange network and charge heater and is then fed to the flash zone at the bottom of the column. Stripping steam is also added at the bottom of the column to provide additional vapor flow. Products with different boiling ranges are withdrawn from the column. The intermediate products

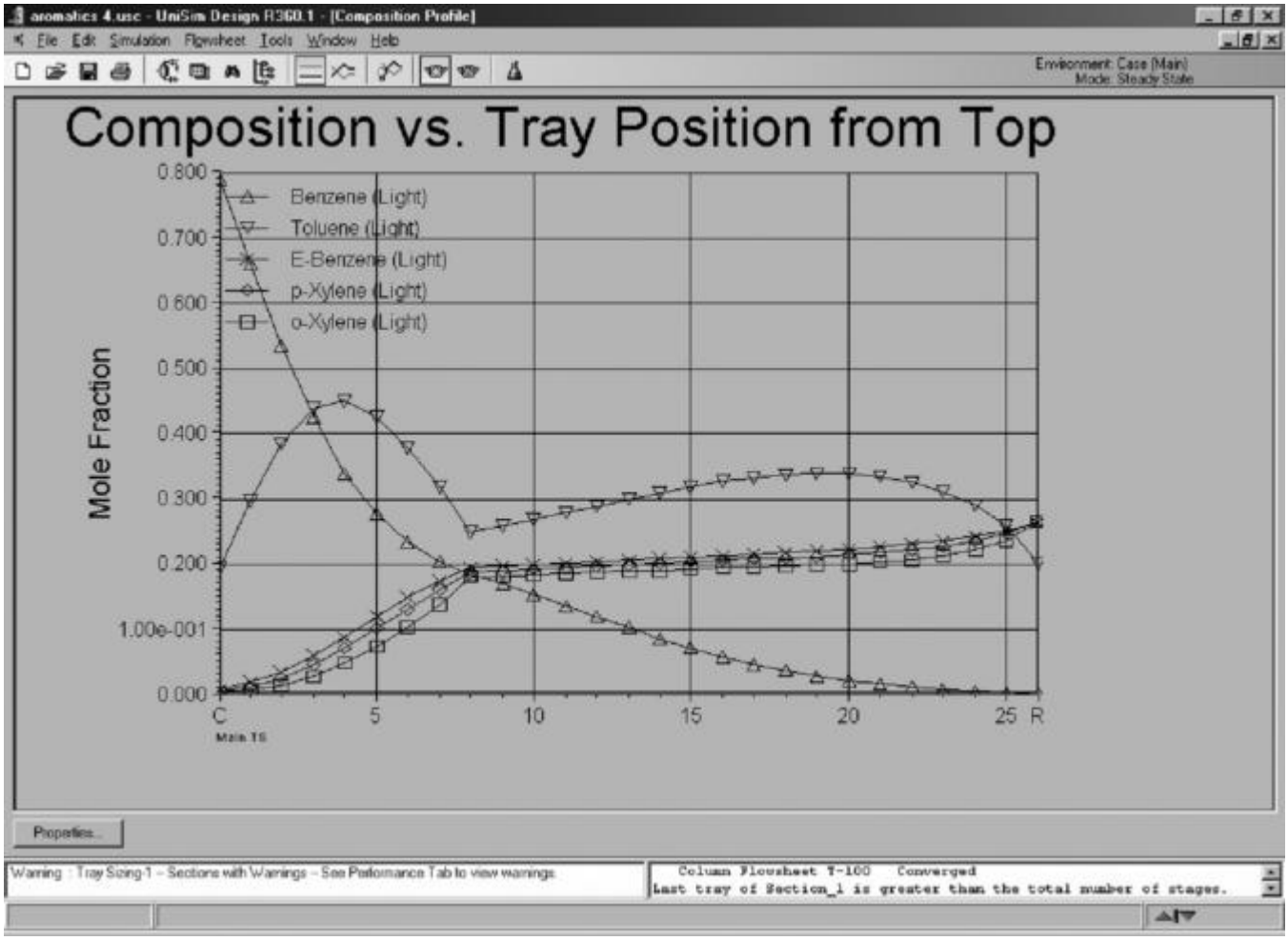


FIG. 4.14 Too few trays: Toluene recovery 24.5%.

are withdrawn from the bottom of side stripper columns, so as to minimize loss of lighter products in the side stream. Although the exact distillation ranges can vary depending on the local fuels specifications and the sophistication of the refinery, the typical products taken in a crude oil distillation unit are (from the bottom up):

1. Atmospheric residue oil (Residue), containing compounds that boil above about 340 °C (650 °F). This is normally sent to a vacuum distillation unit to recover more light products, but parts of it may be blended into high sulfur fuels such as heating oil or bunker fuel (marine fuel).
2. Atmospheric gas oil (AGO), containing compounds that boil in the range 275 °C to 340 °C (530 °F to 650 °F). This material is too high boiling for use as a transportation fuel and is usually sent to a hydrocracker or FCC unit for conversion to lighter products.
3. Heavy distillate (straight-run distillate [SRD]), containing compounds that boil in the range 205 °C to 275 °C (400 °F to 530 °F). This material is hydrotreated to remove sulfur compounds and can then be blended into heating oils and diesel fuels for trucks, railroad engines, and off-road applications such as tractors and mining equipment.
4. Light distillate (straight-run kerosene [SRK]), containing compounds that boil in the range of 175 °C to 230 °C (350 °F to 450 °F). Light distillate is hydrotreated to remove sulfur and can then be blended into jet fuel or sold as kerosene (sometimes called *paraffin*) for lamp and cooking fuel.
5. Naphtha, boiling in the range from 25 °C to 205 °C (80 °F to 400 °F). Naphtha is usually sent to an additional column for separation into a light naphtha boiling below 80 °C (180 °F) and a heavy naphtha. Heavy naphtha has the right boiling range for gasoline but usually has a very low octane number. It is typically upgraded by catalytic reforming using noble metal catalysts to increase the concentration of aromatic hydrocarbons in the naphtha and raise the octane number. Catalytic reforming is also the first step in the production of aromatic hydrocarbons for petrochemicals manufacture. Light naphtha also boils in a suitable range for blending into gasoline and often has

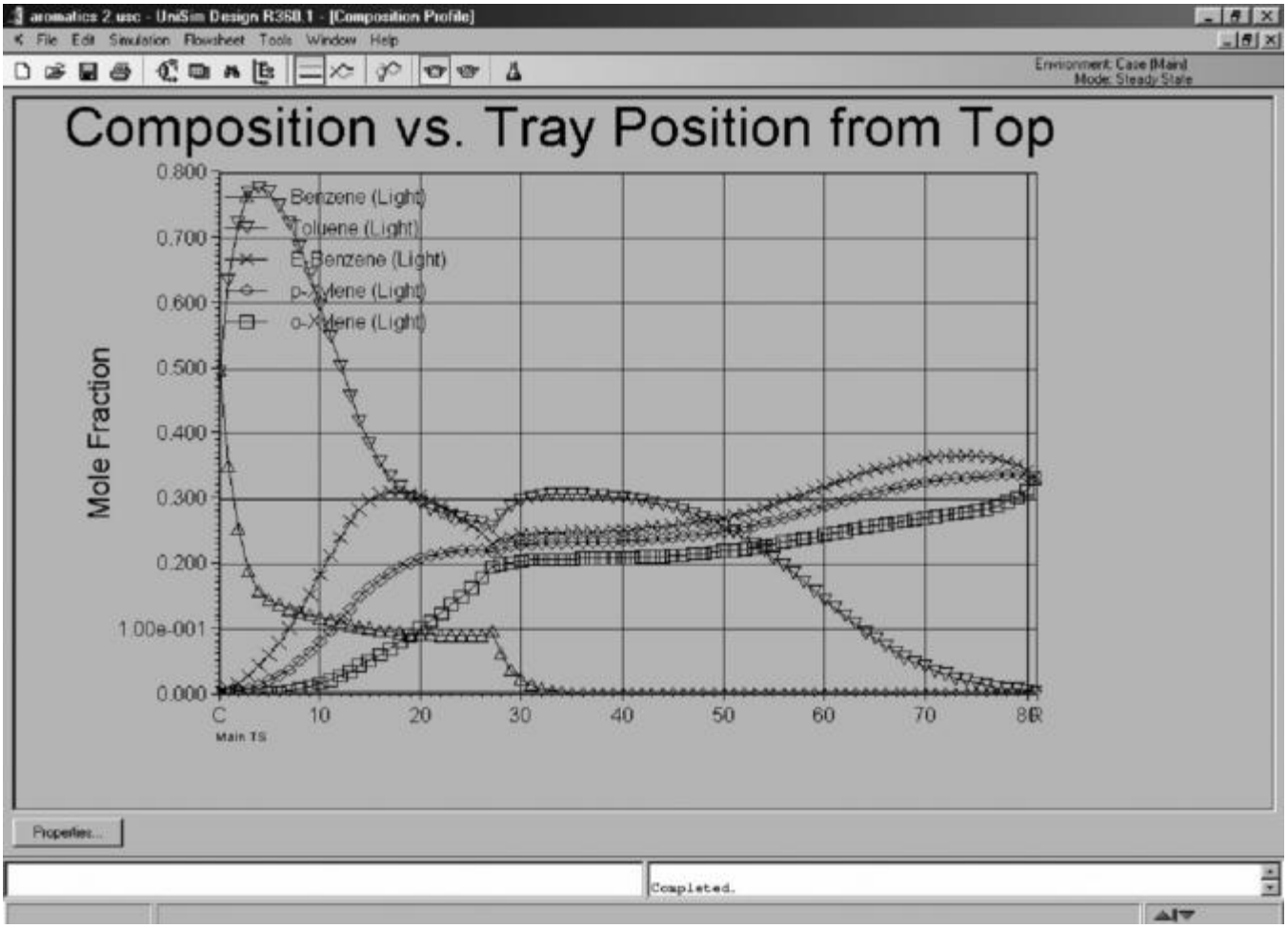


FIG. 4.15 Optimized column profiles.

an acceptable octane number. It is usually treated to oxidize odiferous mercaptan sulfur compounds. Light naphtha is also widely used as a petrochemical feedstock for steam cracking to produce olefin compounds such as ethylene and propylene.

6. The overhead product of the crude unit contains hydrogen, methane, carbon dioxide, hydrogen sulfide, and hydrocarbons up to butanes and some pentanes. It is usually sent to a set of distillation columns known as a *saturate gas plant* for recovery of propane and butane for sale. The lighter gases are then used as refinery fuel.

The design of refinery fractionation columns can be complex. The pump-around streams function as intermediate condensers and remove surplus heat from the column. This heat is usually recovered by heat exchange with the cold crude oil feed. Oil refineries are often designed to handle many different crude oils with different boiling assays. The refinery may make different product slates at different times of the year or in response to market conditions. The crude oil distillation and associated heat-exchange network must be flexible enough to handle all of these variations, while still achieving tight specifications on the boiling point curves of every product.

Column sizing

The rigorous column models allow the design engineer to carry out tray sizing and hydraulics calculations for the basic types of distillation trays and for some types of random and structured packing. Different commercial simulators use different tray sizing correlations, but they all follow a method similar to that described in Chapter 17.

The tray sizing tools are not always enabled when running the distillation models. In some of the simulation programs, the design engineer must enable a tray sizing program and/or enter default values for tray type and tray spacing before the sizing algorithm will work properly. If the column diameter does not change when the reflux rate is significantly changed (or if all the columns in the simulation appear to have the same diameter), then the designer should check to make sure that the tray sizing part of the program is properly configured.

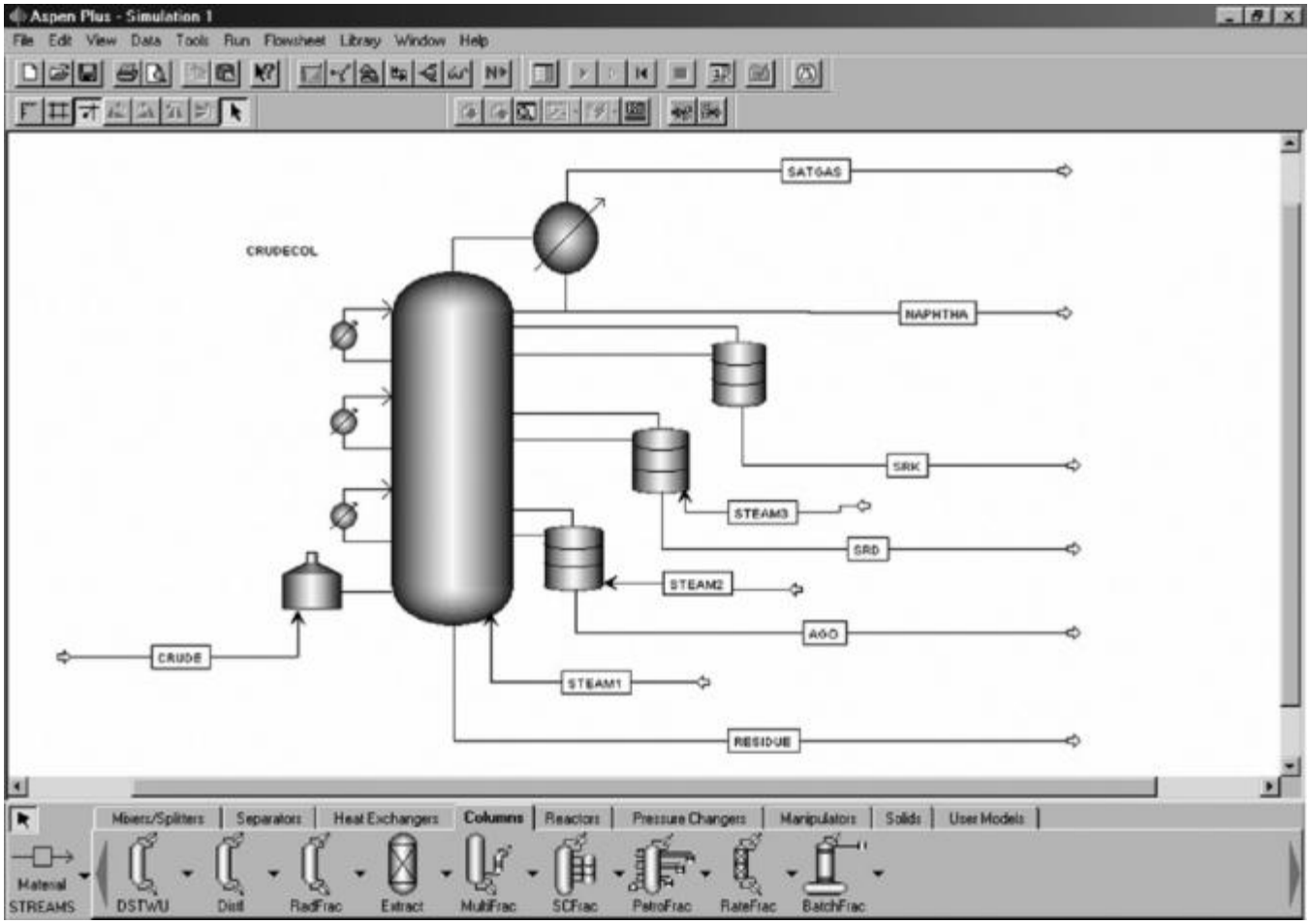


FIG. 4.16 Crude oil fractionation.

The tray sizing options in the simulators are restricted to standard internals such as sieve trays, valve trays, bubble-cap trays, random packings, and structured packings. They do not include high-capacity trays, high-efficiency trays, or the latest packing designs. When designing a column that has many stages or a large diameter, it is always worth contacting the column internals vendors for estimates, as use of high-capacity, high-efficiency internals can lead to substantial savings. Advanced internals are also usually used when revamping an existing column to a higher throughput or tighter product specifications.1

The design engineer should always allow for tray inefficiency when using column sizing tools in conjunction with an equilibrium-stage model. Failure to do so would underpredict the number of stages and hence have an impact on the column pressure drop and hydraulics. Estimation of stage efficiency is discussed in Chapter 17. For initial design purposes, a stage efficiency of 0.7 to 0.8 is usually used. For detailed design, stage efficiencies depend on the type of tray used and are often provided by the column internals vendor.

The design engineer must remember to allow a suitable design factor or design margin when sizing columns. Design factors are discussed in Section 1.6. It may be necessary to create two versions of the flowsheet. One version will have the design basis flow rates for producing the mass and energy balances, and the second will have flow rates that are 10% larger for purposes of sizing equipment.

The simulation of distillation processes is discussed in more detail by Luyben (2013).

Example 4.6

Design a distillation column to separate 225 metric tons per hour of an equimolar mixture of benzene, toluene, ethylbenzene, paraxylene, and orthoxylene with minimum total annualized cost. The feed is a saturated liquid at 330 kPa. The recovery of toluene in the distillate should be greater than 99%, and the recovery of ethylbenzene in the bottoms should be greater than 99%.

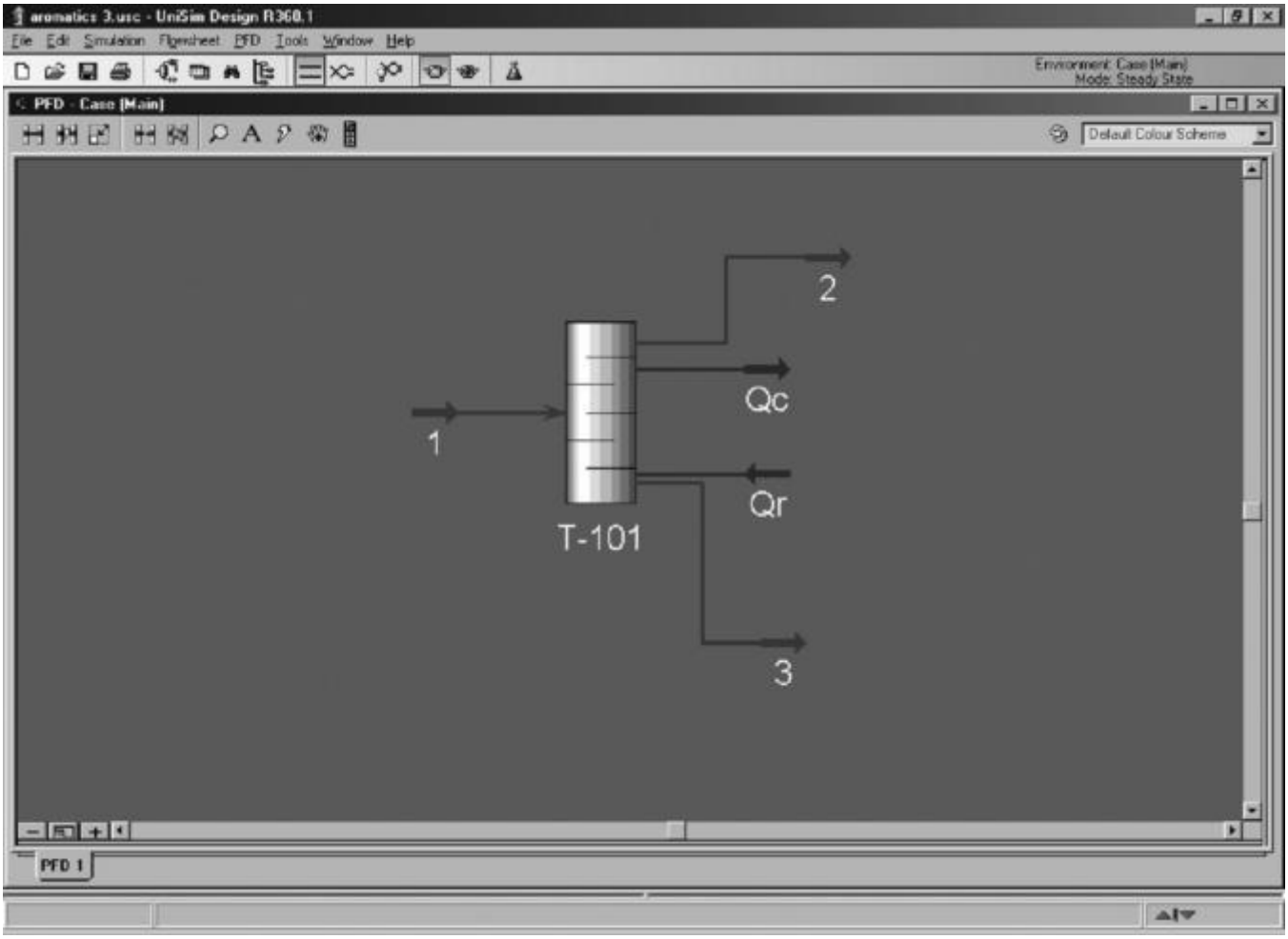


FIG. 4.17 Shortcut distillation.

In this example, a column simulation should be set up using a shortcut model. The shortcut model results will be used to initialize a rigorous model in the example that follows. Determine:

1. The minimum reflux ratio
2. The minimum number of trays
3. The actual number of trays when the reflux is 1.15 R_{min}
4. The optimum feed tray

Solution

This problem was solved using UniSim Design. The problem was set up as a shortcut column, as shown in Fig. 4.17.

UniSim Design requires the designer to specify the mole fraction of the light key component in the bottoms and the heavy key component in the distillate. We have an equimolar feed, so if we take a basis of 100 mol/h of feed, then the molar flow rate of each component is 20 mol/h. A 99% recovery of each key component corresponds to allowing 0.2 mol/h of that component into the other stream. The mole fractions are then:

$$\text{Ethylbenzene in distillate} = 0.2/40 = 0.005$$

$$\text{Toluene in bottoms} = 0.2/60 = 0.00333$$

When these are entered into the shortcut column as specifications, the minimum reflux is calculated to be $R_{\text{min}} = 2.130$. The actual reflux ratio can then be specified as $2.13 \times 1.15 = 2.45$, as shown in Fig. 4.18.

The shortcut column results are shown in Fig. 4.19. The minimum number of stages is calculated as 16.4, which should be rounded up to 17. The actual number of trays required is 39, with feed at stage 18.

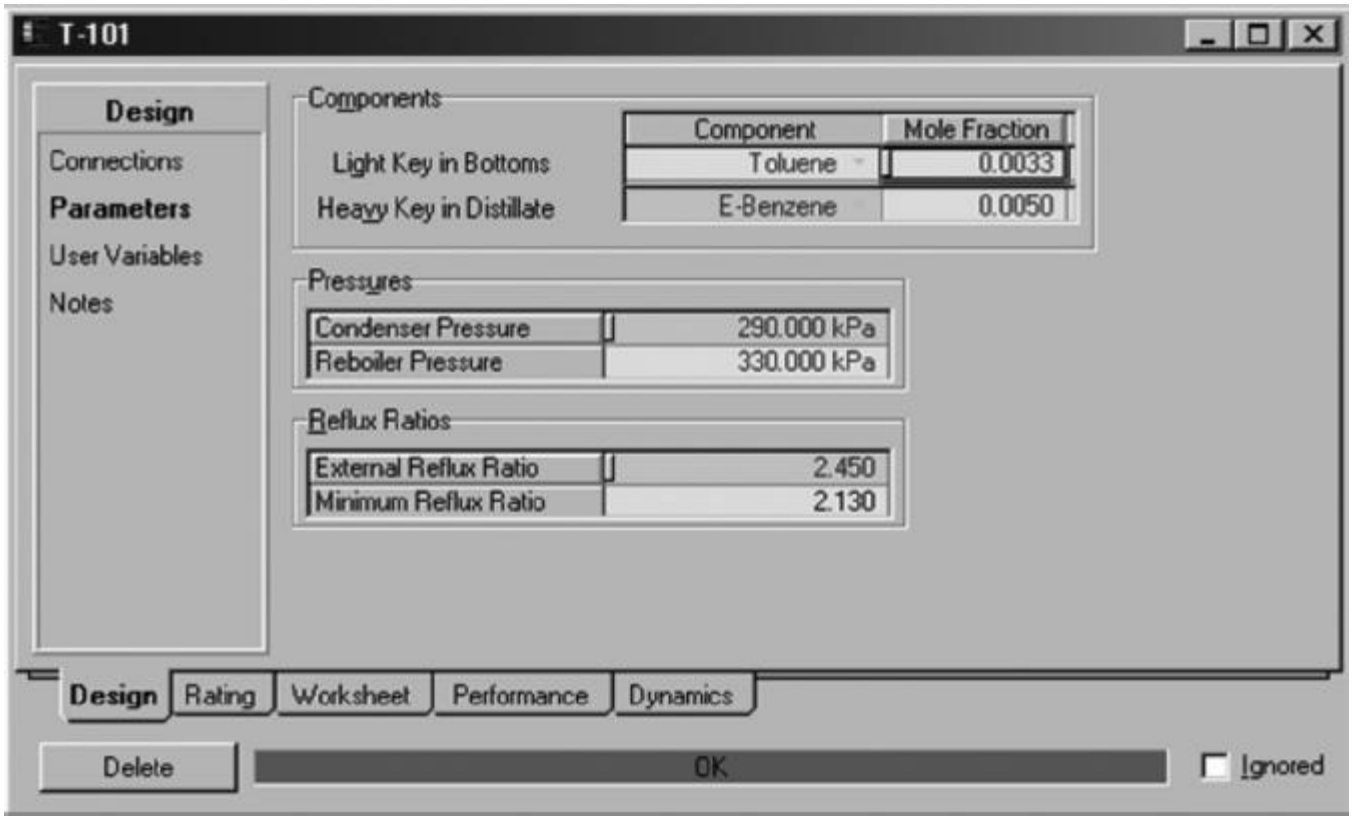


FIG. 4.18 Shortcut column specifications.

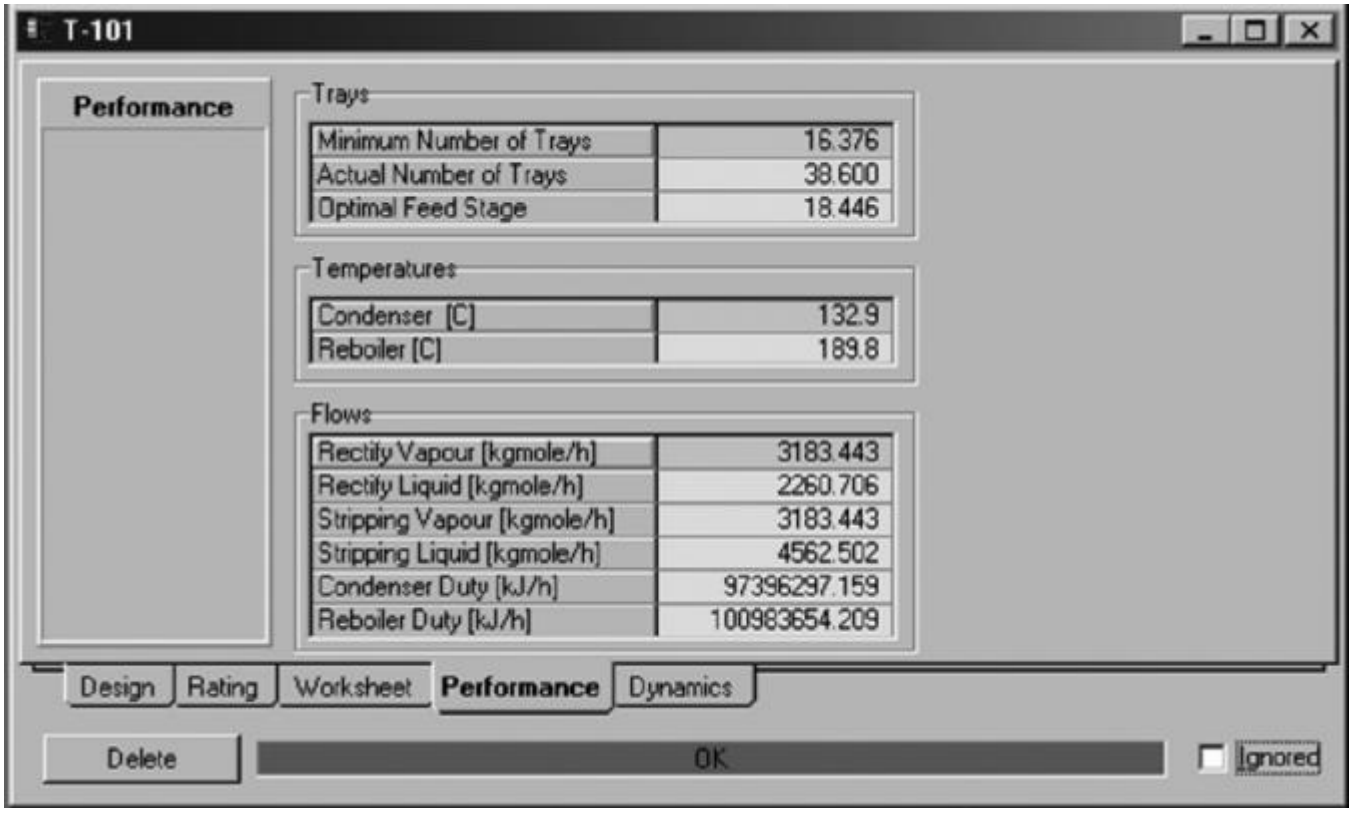


FIG. 4.19 Shortcut column results.

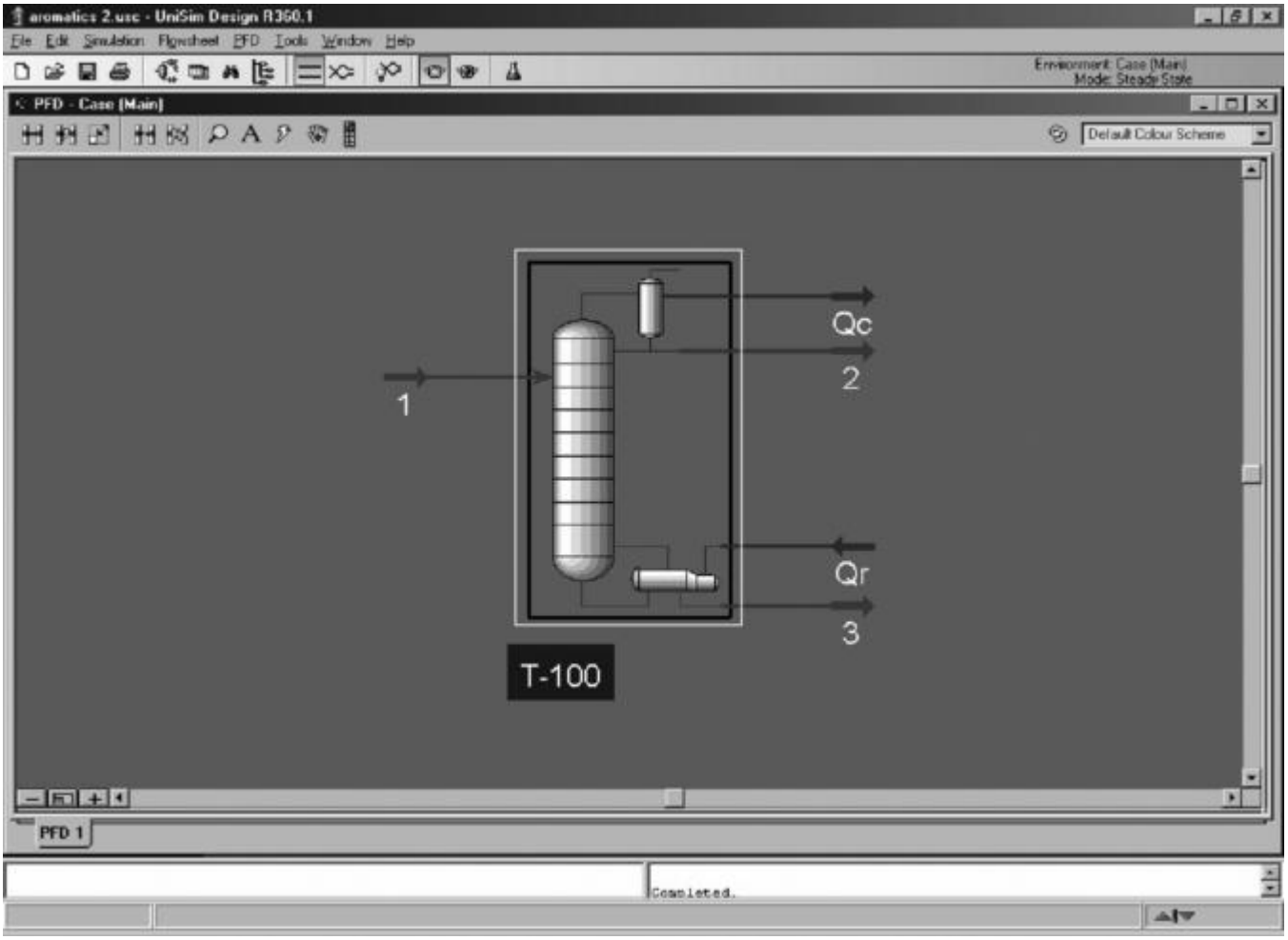


FIG. 4.20 Rigorous distillation.

Example 4.7

Continuing the problem defined in Example 4.6, use a rigorous simulation to carry out tray sizing and estimate the required column diameter.

Solution

Since we are now sizing the column, the first step is to increase the flow rate to allow for a design factor. The process design basis is 225 metric tons per hour of feed. The equipment design should include at least a 10% safety factor, so the equipment design basis was set at 250 metric tons per hour of feed (rounding up from 247.5 for convenience). This flow rate is used in simulating the process for the purpose of sizing equipment, but energy consumption must be based on the reboiler and condenser duties expected for a 225 t/h feed rate.

Fig. 4.20 shows the rigorous column simulation. UniSim Design allows the designer to enter any two specifications for the column, so instead of entering the reflux ratio as a specification, we can enter the required recoveries and provide the value of reflux ratio found in the shortcut model as an initial estimate, as shown in Fig. 4.21.

The column converges quickly with the good estimate provided from the shortcut model. The column profiles can be checked by selecting the "performance" tab in the column environment and then selecting "plots" from the menu on the left and "composition" from the list of possible plots, as shown in Fig. 4.22. This generates composition profiles like those presented in Figs. 4.10 to 4.15.

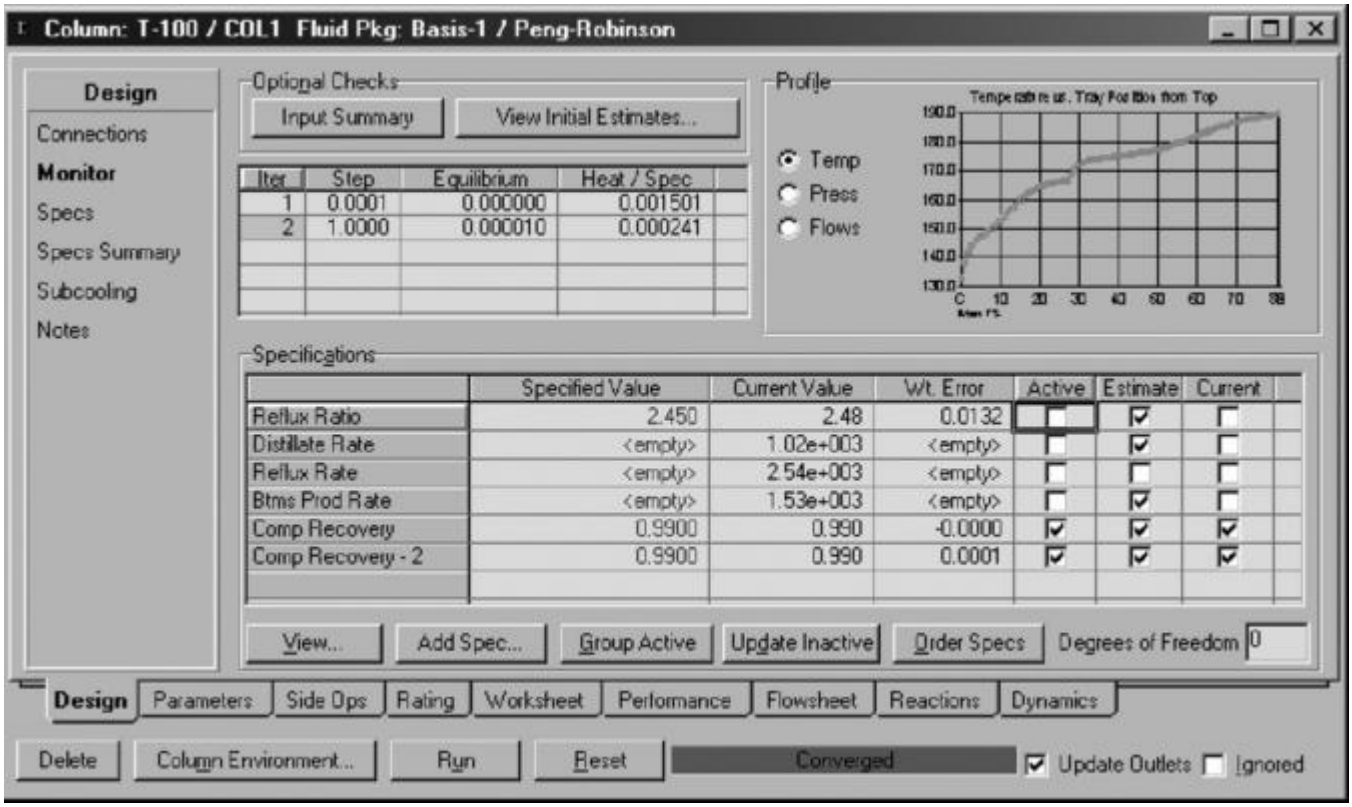


FIG. 4.21 Rigorous column specifications.

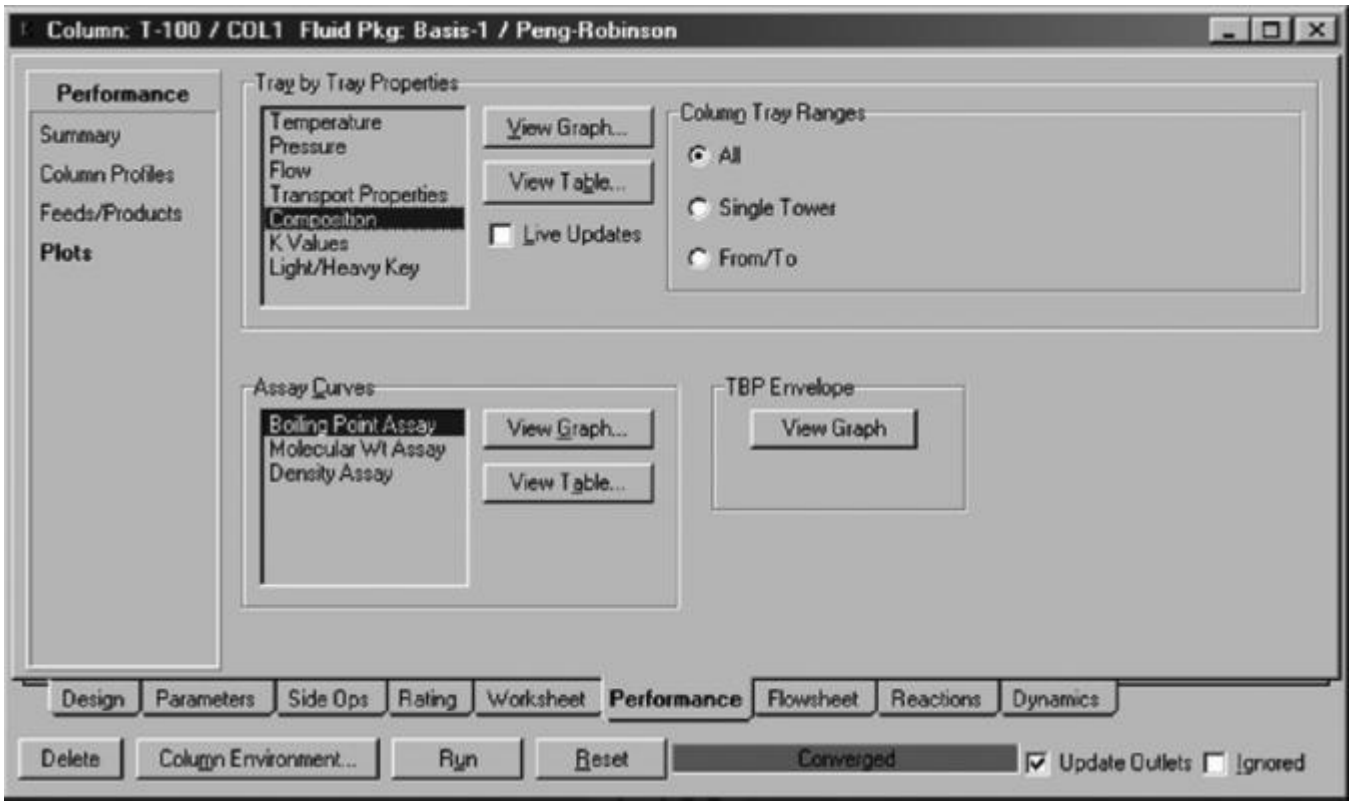


FIG. 4.22 Generating column profiles.

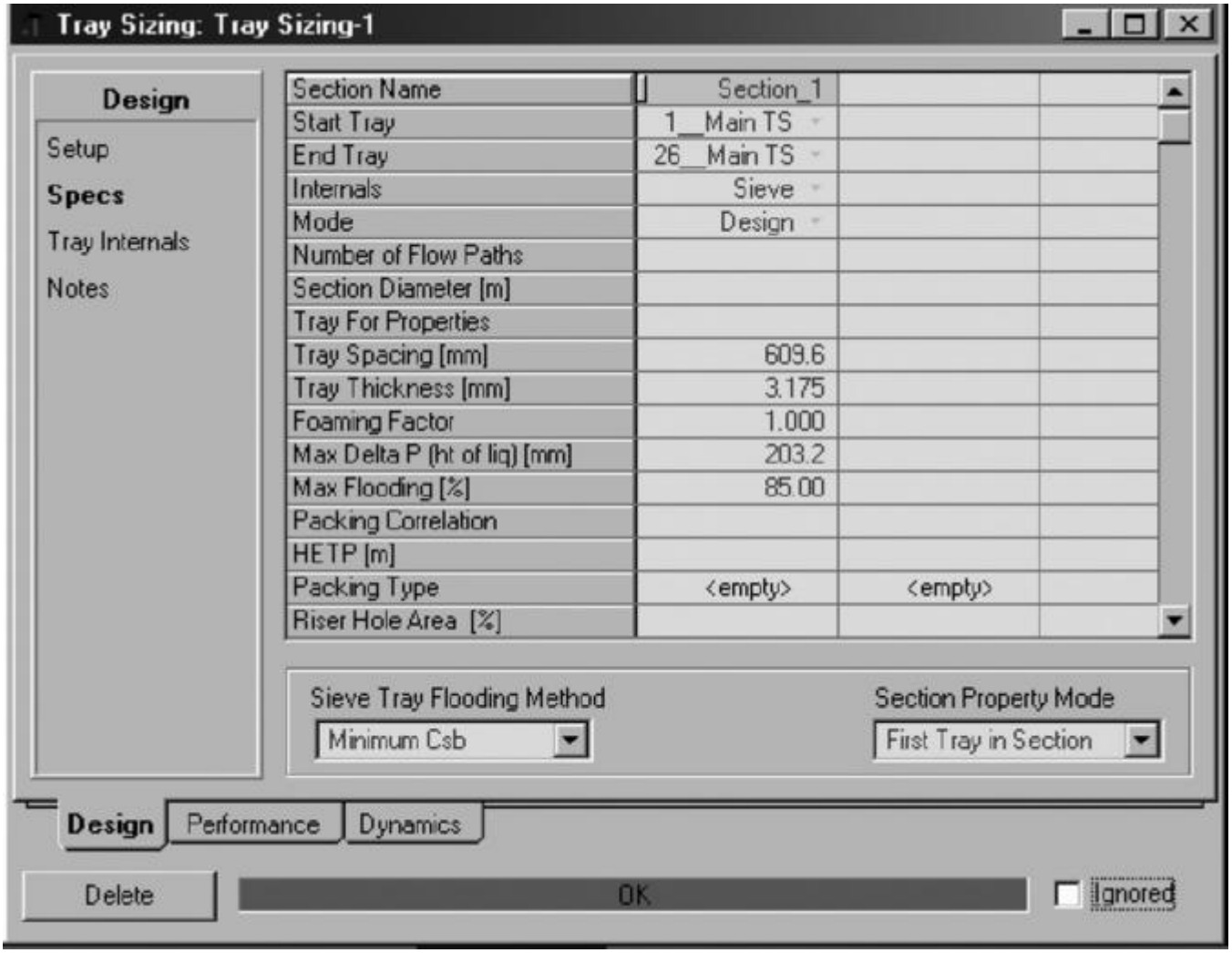


FIG. 4.23 Default tray sizing options.

To size the trays in UniSim Design, the tray sizing utility must be activated (from the tools menu via tools/utilities/tray sizing). When sieve trays are selected with the default spacing of 609.6 mm (2 ft) and the other default parameters shown in Fig. 4.23, then the results in Fig. 4.24 are obtained. The column diameter is found to be 4.42 m (14.5 ft).

The data on column size, number of trays, reboiler, and condenser duty can then be extracted from the simulation and put into a cost model or spreadsheet to carry out optimization of the total annual cost of production. The results of the optimization are described in Example 12.1.

4.5.3 Other separations

Other multistage vapor–liquid separations such as absorption and stripping can be modeled using variations of the rigorous distillation models, as can multistage liquid–liquid extraction.

Single-stage liquid–liquid or vapor–liquid separation can be modeled as a flash vessel, but some caution is needed. The simulation programs assume perfect separation in a flash unless the designer specifies otherwise. If there is entrainment of droplets or bubbles, the outlet compositions of a real flash vessel will be different from those

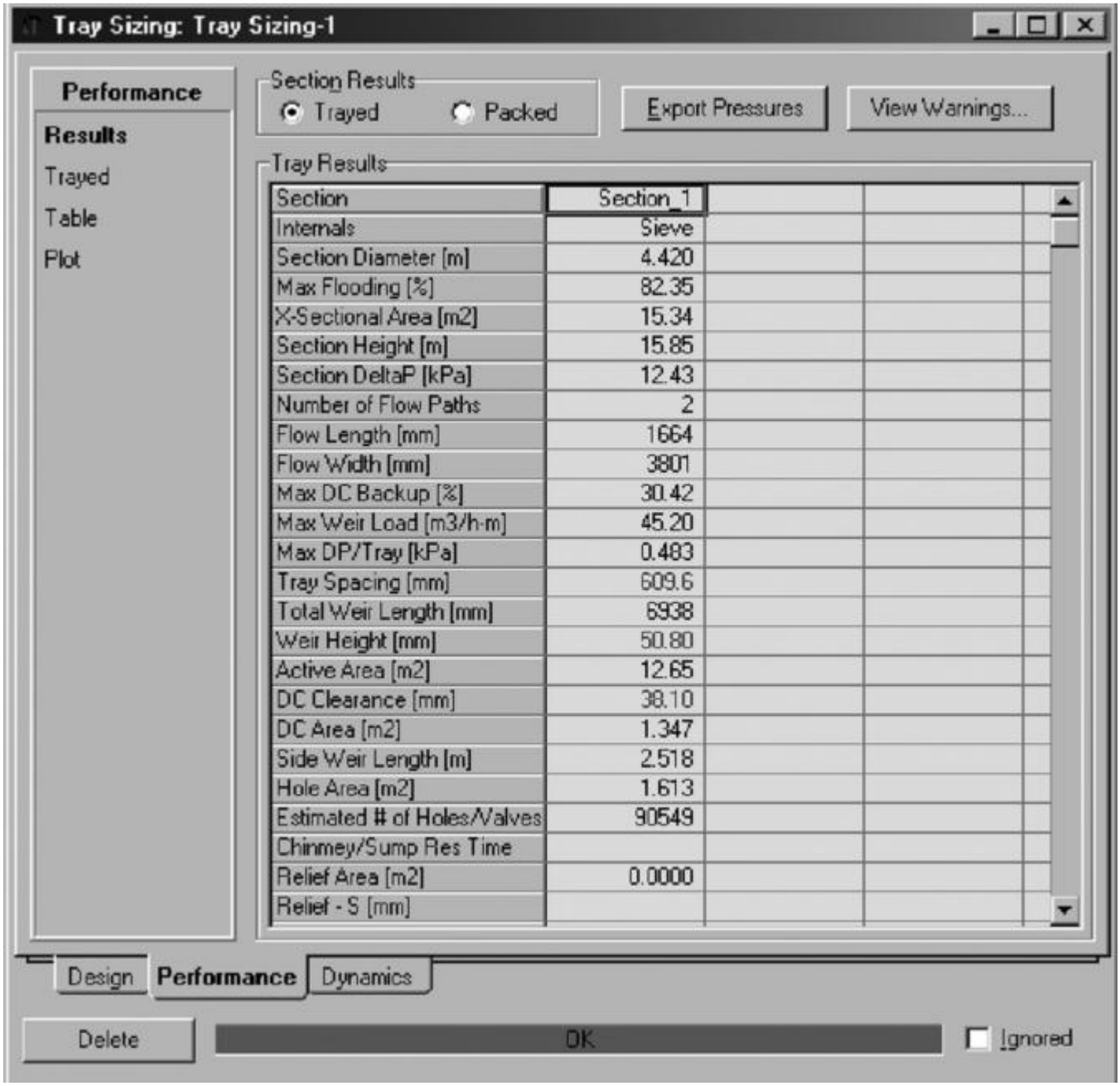


FIG. 4.24 Tray sizing results.

predicted by the simulation. If the flash is critical to process performance, the designer should make an allowance for entrainment. Most of the simulation programs allow the designer to specify a fraction of each phase that is entrained with the other phases. This is illustrated in Fig. 4.25, which shows the data entry sheet for entrained flows for UniSim Design. In UniSim Design, the entrained fractions are entered on the "Rating" tab of the flash model window. Users can also use built-in correlation models with their specified information such as vessel dimensions and nozzle locations. More sophisticated real separator modeling can be found in the three-phase separator model in UniSim Design. The fraction that is entrained depends on the design of the vessel, as described in Chapter 16.

Most of the simulators contain several models for fluid–solid separation. These models can be used to manipulate the particle size distribution when solids are present.



FIG. 4.25 Flash model with entrainment.

None of the commercial process simulators contains a good library model for adsorptive separations or membrane separations at the time of writing. These separation methods are important for gas–gas separations, chromatographic separations, and size exclusion or permeation-based separations and are described in more detail in Chapter 16. All of these processes must be modeled using component splitters, as described next.

Component splitter models

A component splitter is a subroutine in the simulation that allows a set of components from a stream to be transferred into another stream with a specified recovery. Component splitters are convenient for modeling any separation process that cannot be described using one of the library models. Examples of real operations that are usually modeled as component splitters include:

- Pressure swing adsorption
- Temperature swing adsorption
- Chromatography
- Simulated moving bed adsorption
- Membrane separation
- Ion exchange
- Guard beds (irreversible adsorption)

When a component splitter is used in a model, it is a good practice to give the splitter a label that identifies the real equipment that is being modeled.

Component splitters are sometimes used in place of distillation columns when building simple models to provide initial estimates for processes with multiple recycles. There is little advantage to this approach compared with using

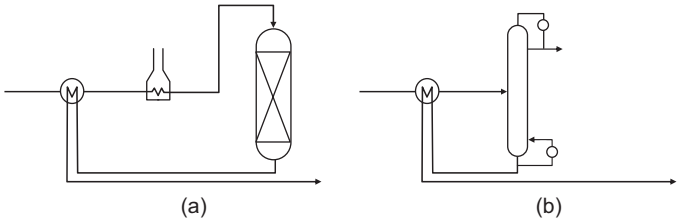


FIG. 4.26 Common feed heating schemes. (a) Feed-effluent exchange. (b) Feed-bottoms exchange.

shortcut distillation models, as the component splitter will not calculate the distribution of nonkey components unless a recovery is entered for each. Estimating and entering the recoveries for every component is difficult and tedious, and poor estimates of recoveries can lead to poor estimates of recycle flows, so the use of component splitters in this context effectively adds another layer of iteration to the model.

4.5.4 Heat exchange

All of the commercial simulators include models for heaters, coolers, heat exchangers, fired heaters, and air coolers. The models are easy to configure, and the only inputs that are usually required on the process side are the estimated pressure drop and either the outlet temperature or the duty. A good initial estimate of pressure drop is 0.3 to 0.7 bar (5 to 10 psi).

The heater, cooler, and heat exchanger models allow the design engineer to enter estimates of film transfer coefficients and hence calculate the exchanger area. As with distillation columns, the designer must remember to add a design factor to the sizes predicted by the model. Design factors are discussed in Section 1.6.

Problems often arise when using heat exchanger models to simulate processes that have a high degree of process-to-process heat exchange. Whenever a process-to-process heat exchanger is included in a simulation, it sets up an additional recycle of information; consequently, an additional loop must be converged. A common situation is where the effluent from a reactor or the bottoms from a distillation column is used to pre-heat the reactor or column feed, as illustrated in Fig. 4.26. If these process flow schemes are simulated using heat exchangers, a recycle of energy is set up between the product and the feed. This recycle must be converged every time the flowsheet is calculated (i.e., at every iteration of any other recycle loop in the process). If more than a few of these exchangers are present, the overall flowsheet convergence can become difficult.

Instead, it is usually a good practice to model the process using only heaters and coolers and then set up subproblems to model the heat exchangers. This facilitates data extraction for pinch analysis, makes it easier for the designer to recognize when exchangers might be internally pinched or have low F factors (see Chapter 19), and improves convergence.

Another problem that is often encountered when simulating heat exchangers and heat-exchange networks is temperature cross. A temperature cross occurs when the cold stream outlet temperature is hotter than the hot stream outlet temperature (see Section 19.6). When temperature cross occurs, many types of shell and tube heat exchangers give a very poor approximation of counter-current flow, and consequently have low F factors and require large surface areas. In some of the commercial simulation programs, the heat exchanger models will indicate if the F factor is low. If this is the case, the designer should split the exchanger into several shells in series so that temperature cross is avoided. Some of the simulation programs allow the designer to plot profiles of temperature versus heat flow in the exchanger. These plots can be useful in identifying temperature crosses and internal pinches.

Example 4.8

A mixture of 100 kgmol/h of 80 mol% benzene and 20 mol% ethylene at 40 °C and 100 kPa is fed to a feed effluent exchanger, where it is heated to 300 °C and fed to a reactor. The reaction proceeds to 100% conversion of ethylene, and the reactor products are withdrawn, cooled by heat exchange with the feed, and sent for further processing. Estimate the outlet temperature of the product after heat exchange and the total surface area required if the average heat transfer coefficient is 200 $Wm^{-2}K^{-1}$.

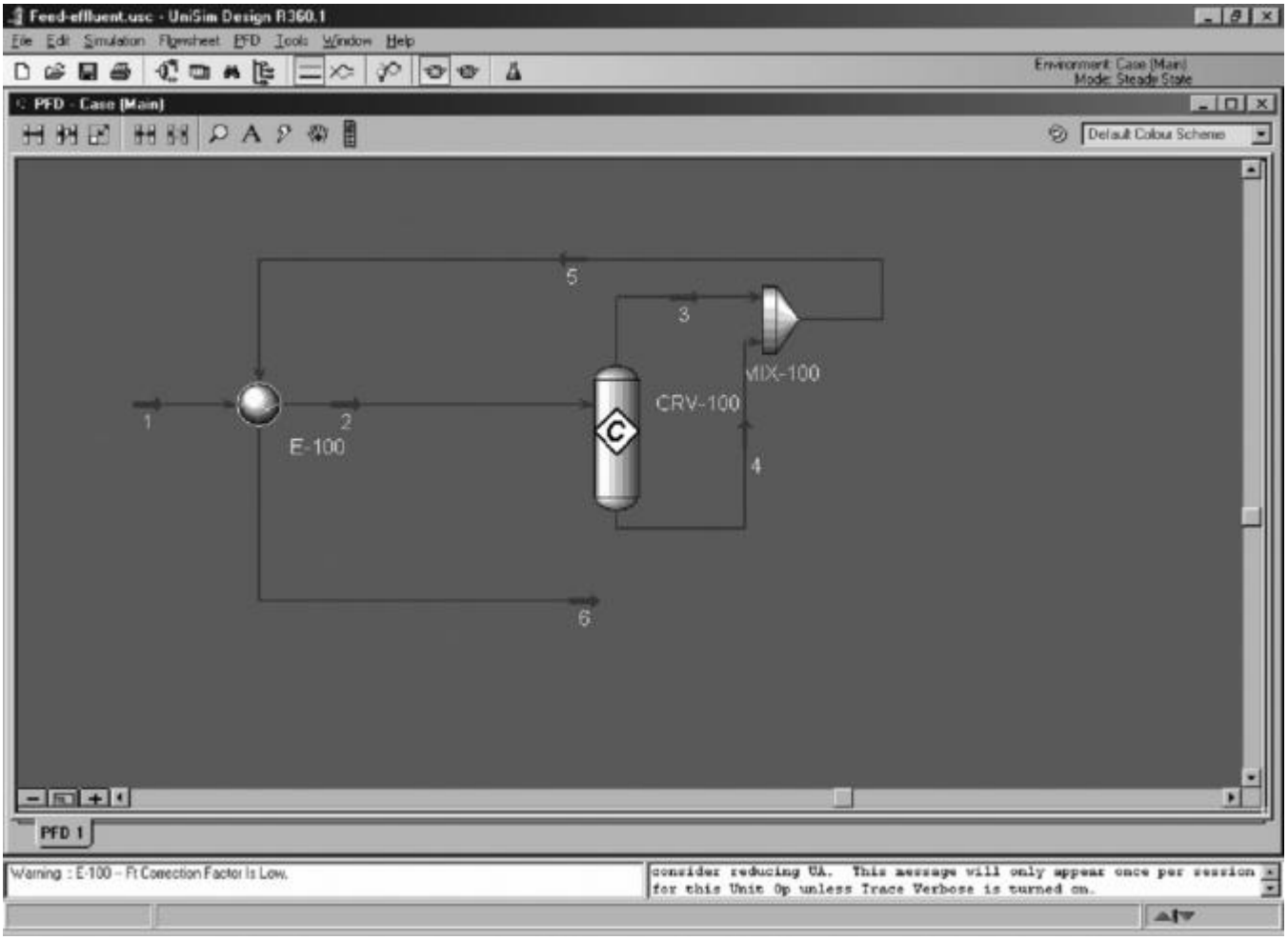


FIG. 4.27 Feed-effluent heat exchange model for Example 4.8.

Solution

This problem was solved using UniSim Design. The reaction goes to full conversion, so a conversion reactor can be used. The simulation model is shown in Fig. 4.27.

When the temperature at the outlet of the exchanger on the feed side is specified, the duty of the exchanger is defined and there is no recycle of information. The model thus solves very quickly, but it is necessary to check the results to see that the exchanger design makes sense.

The outlet temperature of the product (stream 6) is found to be 96.9 °C, so there is enough heat in the product mixture to give an approach temperature of nearly 60 °C, which seems perfectly adequate. If we open the exchanger worksheet, though, there is a warning that the F factor is too low. Fig. 4.28 shows the exchanger worksheet, and the F factor is only 0.2, which is not acceptable. When we examine the temperature–heat duty plot shown in Fig. 4.29 (generated from the Performance tab of the exchanger worksheet), it is clear that there is a substantial temperature cross. This temperature cross causes the exchanger to have such a low F factor and gives a UA value of 78.3×10^3 WK^{-1}, where U is the overall heat transfer coefficient in $Wm^{-2}K^{-1}$ and A is the area in m^2.

If $UA = 78.3 \times 10^3$ WK^{-1} and $U = 200$ $Wm^{-2}K^{-1}$, then the exchanger area is $A = 392$ m^2. This would be a feasible size of exchanger, but is large for the duty and is not acceptable because of the low F factor. We should add more shells in series.

By examining the temperature–heat duty plot in Fig. 4.29, we can see that if we break the exchanger into two shells, with the first shell heating the feed up to the dew point (the kink in the lower curve), then the first shell will not have a temperature cross. This design corresponds to an outlet temperature of about 70 °C for the first exchanger. The second exchanger would

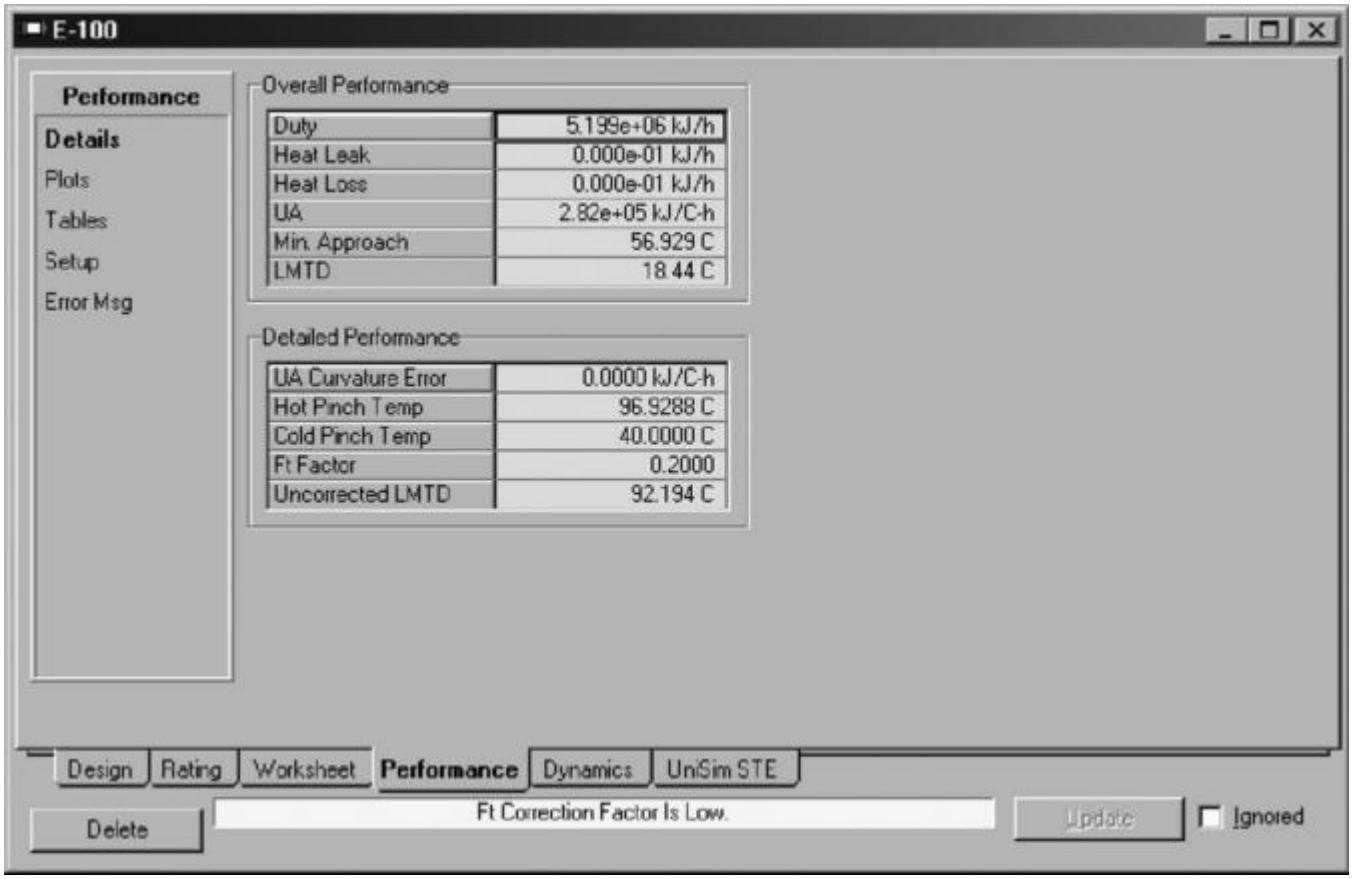


FIG. 4.28 Exchanger worksheet for a single-shell design.

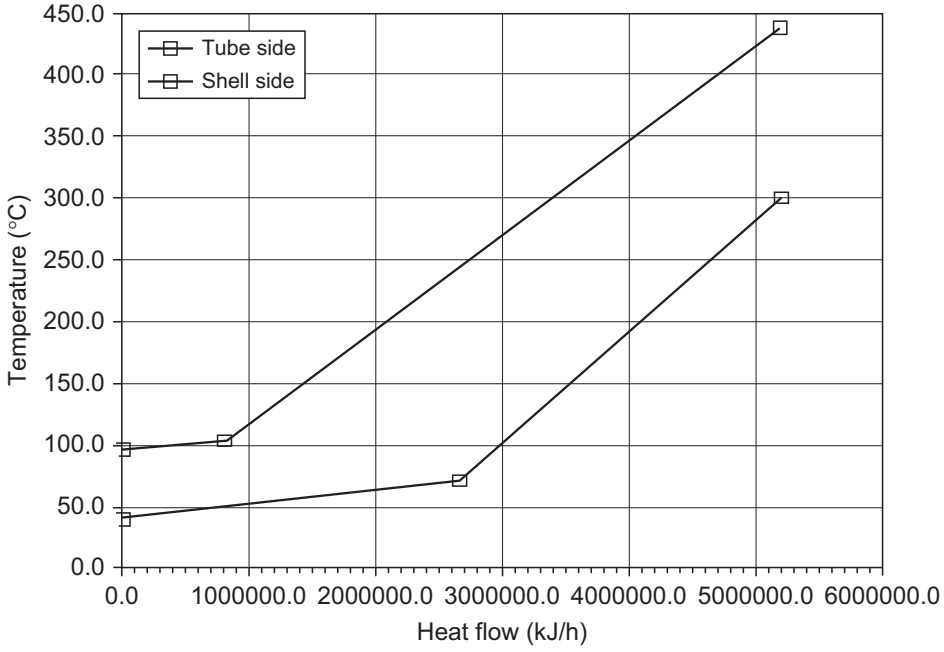


FIG. 4.29 Temperature–heat flow plot for a single-shell design.

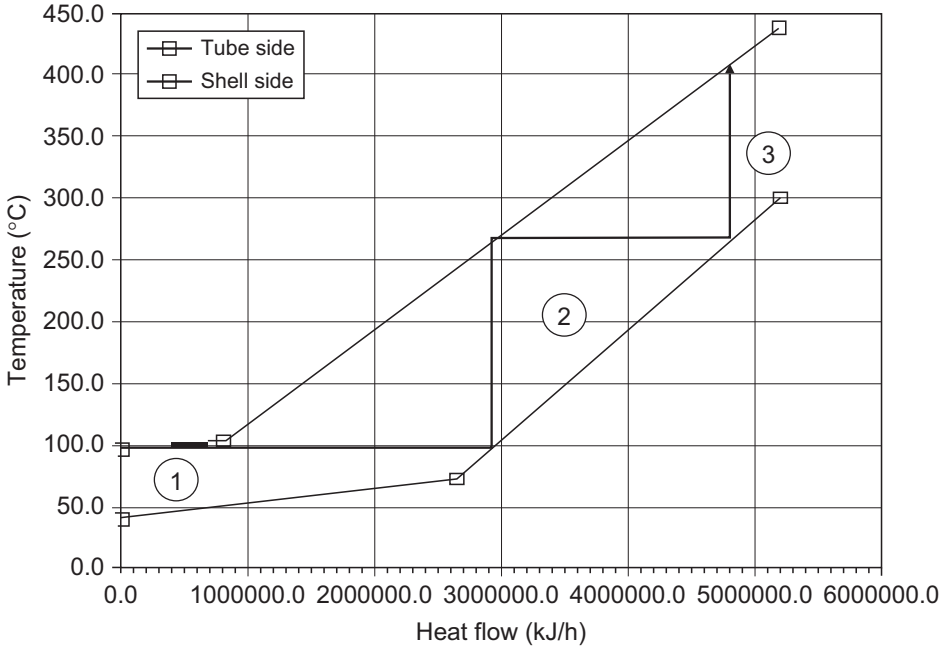


FIG. 4.30 Stepping between heat profiles to avoid temperature cross.

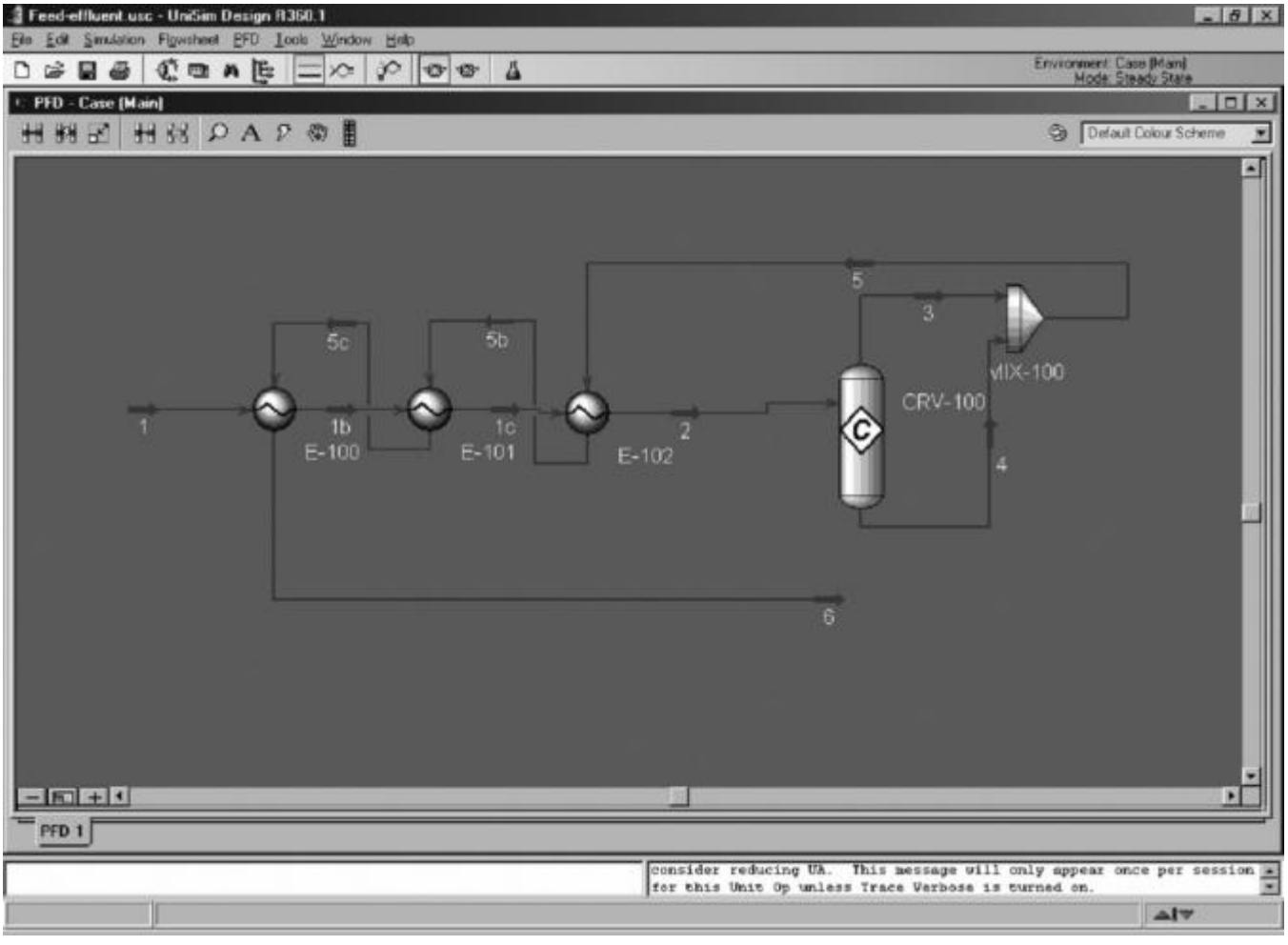


FIG. 4.31 Feed–effluent heat exchange with three shells in series.

still have a temperature cross though. If we break this second exchanger into two more exchangers, then the temperature cross is eliminated. We thus need at least three heat exchangers in series to avoid the temperature cross. This result could have been obtained by "stepping off" between the temperature–heat duty plots, as illustrated in Fig. 4.30.

Fig. 4.31 shows a modified flowsheet with two additional heat exchangers added in series. The outlet temperature of the second exchanger was specified as 200 °C to divide the duty of the second and third exchangers roughly equally. The results are given in Table 4.7. Temperature–heat flow plots for the three exchangers are given in Fig. 4.32.

The modified design achieved a reduction in surface area from 392 m^2 to 68 m^2 at the price of having three shells instead of the original one. More importantly, the modified design is more practical than the original design and is less likely to suffer from internal pinch points. The modified design is not yet optimized. Optimization of this problem is explored in Problem 4.11.

TABLE 4.7 Heat exchanger results

Design case	**Original (single shell)**	**Modified (multiple shell)**		
Exchanger	***E100***	***E100***	***E101***	***E102***
Duty (MW)	1.44	0.53	0.57	0.35
UA (W/K)	78,300	6310	4780	2540
F	0.2	0.93	0.82	0.93
ΔT_{min}	56.9	56.9	134.3	139.7
ΔT_{lmtd}	18.4	83.6	118.7	138.4
A (m^2)	392	32	24	13
Total area (m^2)	392		68	

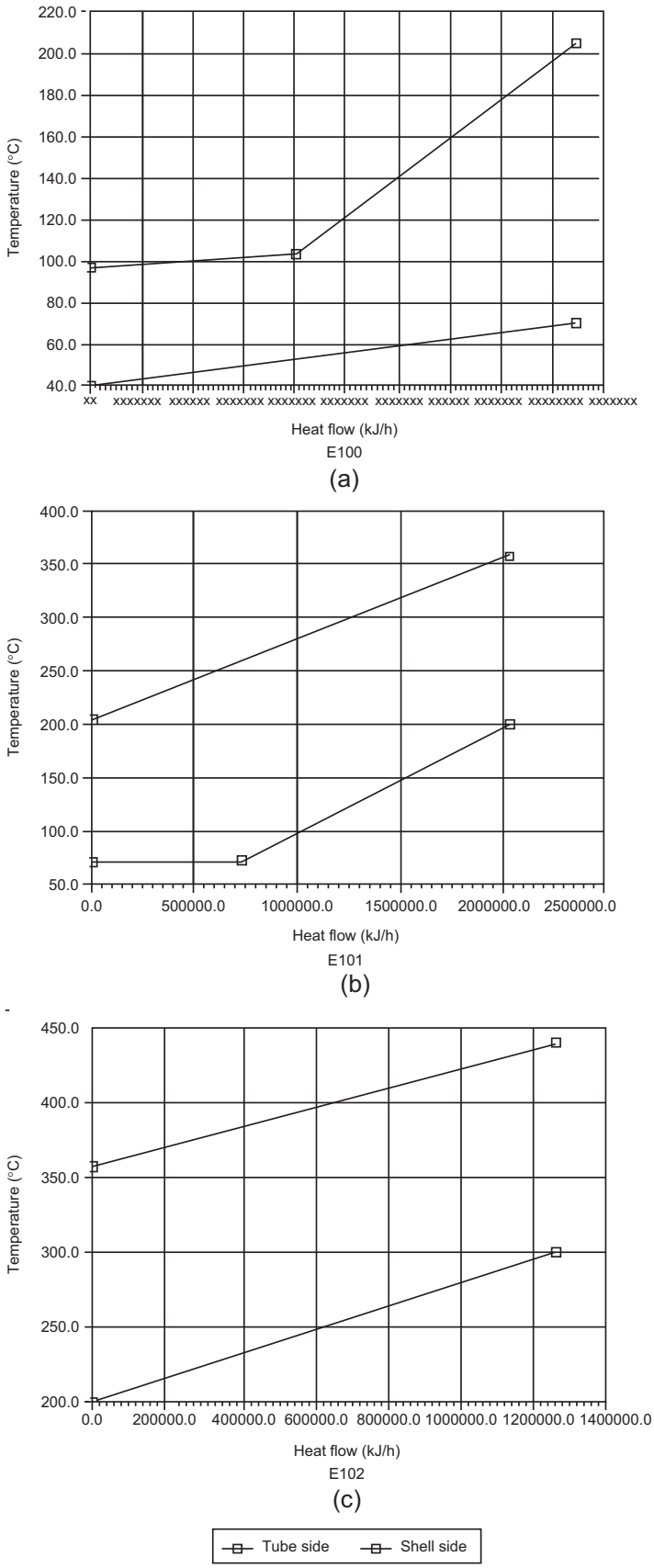


FIG. 4.32 Temperature–heat flow profiles for the three exchangers in series (a) E100, (b) E101, and (c) E102.

4.5.5 Hydraulics

Most of the commercial simulation programs contain models for valves, pipe segments, tees, and elbows. These models can be used to make an initial estimate of system pressure drop for the purposes of sizing pumps and compressors.

If a process hydraulic model is built, care must be taken to specify pressure drop properly in the unit operation models. Rules of thumb are adequate for initial estimates, but in a hydraulic model these should be replaced with rigorous pressure drop calculations. Sufficient allowance must be made for pressure drop across control valves, as discussed in Chapters 5 and 20.

A hydraulic model will not be accurate unless some consideration has been given to plant layout and piping layout. Ideally, the hydraulic model should be built after the piping isometric drawings have been produced, when the designer has a good idea of pipe lengths and bends. The designer should also refer to the piping and instrumentation diagram for isolation valves, flow meters, and other obstructions that cause increased pressure drop. These subjects are discussed in Chapter 5 and Chapter 20.

Care is needed when modeling compressible gas flows, flows of vapor–liquid mixtures, slurry flows, and flows of nonnewtonian liquids. Some simulators use different pipe models for compressible flow. The prediction of pressure drop in multiphase flow is inexact at best and can be subject to very large errors if the extent of vaporization is unknown. In most of these cases, the simulation model should be replaced by a computational fluid dynamics (CFD) model of the important parts of the plant.

4.5.6 Solids handling

The commercial simulation programs were originally developed mainly for petrochemical applications, and none of them has a complete set of solids-handling operations. Although models for filters, crystallizers, decanters, and cyclones are present in most of the simulators, the designer may have to add user models for operations such as:

- hoppers
- belt conveyors
- elevators
- pipe conveyors
- screw conveyors
- kneaders
- extruders
- slurry pumps
- fluidized bed heaters
- fluidized bed reactors
- washers
- flocculators
- spray driers
- prill towers
- rotary driers
- rotary kilns
- belt driers
- centrifuges
- falling film evaporators
- moving bed reactors
- crushers and pulverizers
- jet mills
- ball mills
- agglomerators
- granulators
- tableting presses
- paper machines
- classifiers
- electrostatic precipitators

Because solids are handled in many commodity chemical processes as well as pharmaceuticals, polymers, and biological processes, the simulation software vendors are under pressure from their customers to enhance the capability of the programs for modeling solids operations. This continues to be an area of evolution of the commercial software.

4.6 User models

When the design engineer needs to specify a unit operation that is not represented by a library model and cannot be approximated by a simple model such as a component splitter or a combination of library models, then it is necessary to construct a user model. All of the commercial simulators allow the user to build add-in models of varying sophistication.

4.6.1 Spreadsheet models

Models that require no internal iteration are easily coded as spreadsheets. Most of the simulators offer some degree of spreadsheet capability, ranging from simple calculation blocks to full Microsoft Excel functionality.

In UniSim Design, spreadsheets can be created by selecting the spreadsheet option on the unit operations palette. The spreadsheet is easy to configure and allows data to be imported from streams and unit operations. The functionality of the UniSim Design spreadsheet is rather basic at the time of writing, but is usually adequate for simple input-output models. Values calculated by the spreadsheet can be exported back to the simulation model. The spreadsheet can thus be set up to act as a unit operation. The use of a spreadsheet as a unit operation is illustrated in Example 4.9. Aspen Plus has a similar simple spreadsheet capability using Microsoft Excel, which can be specified as a calculator block (via Data/Flowsheet Options/Calculator). The Excel calculator block in Aspen Plus requires a little more time to configure than the UniSim Design spreadsheet, but at the time of writing it can perform all of the functions available in Microsoft as discussed in Chapter 5 and Chapter 20.

For more sophisticated spreadsheet models, Aspen Plus allows the user to link a spreadsheet to a simulation via a user model known as a USER2 block. The designer can create a new spreadsheet or customize an existing spreadsheet to interact with an Aspen Plus simulation. The USER2 block is much easier to manipulate when handling large amounts of input and output data, such as streams with many components or unit operations that involve multiple streams. The procedure for setting up a USER2 Microsoft Excel model is more complex than using a calculator block, but avoids having to identify every number required from the flowsheet individually. Instructions on how to build USER2 spreadsheet models are given in the Aspen Plus manuals and online help (Aspen Technology, 2001).

4.6.2 User subroutines

Models that require internal convergence are best written as subroutines rather than spreadsheets, as more efficient solution algorithms can be used. Most user subroutines are written in FORTRAN or Visual Basic, though some of the simulators allow other programming languages to be used.

It is generally a good practice to compile and test a user model in a simplified flowsheet or as a stand-alone program before adding it to a complex flowsheet with recycles. It is also a good practice to check the model carefully over a wide range of input values, or else constrain the inputs to ranges where the model is valid.

Detailed instructions on how to write user models to interface with commercial simulation programs can be found in the simulator manuals. The manuals also contain specific requirements for how the models should be compiled and registered as extensions or shared libraries (.dll files in Microsoft Windows). In Aspen Plus, user models can be added as USER or USER2 blocks, following the instructions in the Aspen Plus manuals. In UniSim Design, it is easy to add user models using the User Unit Operation, which can be found on the object palette or under the Flowsheet/Add Operation menu. The UniSim Design User Unit Operation can be linked to any program without requiring an extension file to be registered. The User Unit Operation is not documented in the UniSim Design manual, but instructions on setting it up and adding code are given in the online help.

Example 4.9

A gas turbine engine is fueled with 3000 kg/h of methane at 15 °C and 1000 kPa and supplied with ambient air at 15 °C. The air and fuel are compressed to 2900 kPa and fed to a combustor. The air flow rate is designed to give a temperature of 1400 °C at the outlet of the combustor. The hot gas leaving the combustor is expanded in the turbine. Shaft work produced by the turbine is used to power the two compressors and run a dynamo for generating electricity.

If the efficiency of the compressors is 98% and that of the turbine is 88% and 1% of the shaft work is lost due to friction and losses in the dynamo, estimate the rate of power production and the overall cycle efficiency.

Solution

This problem was solved using UniSim Design.

A gas turbine engine should run with a large excess of air to provide full combustion of the fuel so the combustor can be modeled as a conversion reactor. There is no model for a dynamo in UniSim Design, so the dynamo and shaft losses can be modeled using a spreadsheet operation, as shown in Fig. 4.33.

Fig. 4.33 also illustrates the use of an "Adjust" controller to set the air flow rate so as to give the desired reactor outlet temperature. The specifications for the Adjust controller are shown in Figs. 4.34 and 4.35. The Adjust controller was specified with a minimum air flow rate of 60,000 kg/h to ensure that the solver did not converge to a solution in which the air flow did not give full conversion of methane. The stoichiometric requirement is $3000 \times 2 \times (32 / 16) / 0.21 = 57{,}000$ kg/h of air.

The spreadsheet model of the dynamo is relatively simple, as illustrated in Fig. 4.36. The model takes the turbine shaft work and compressor duties as inputs. The friction losses are estimated as 1% of the turbine shaft work. The friction losses

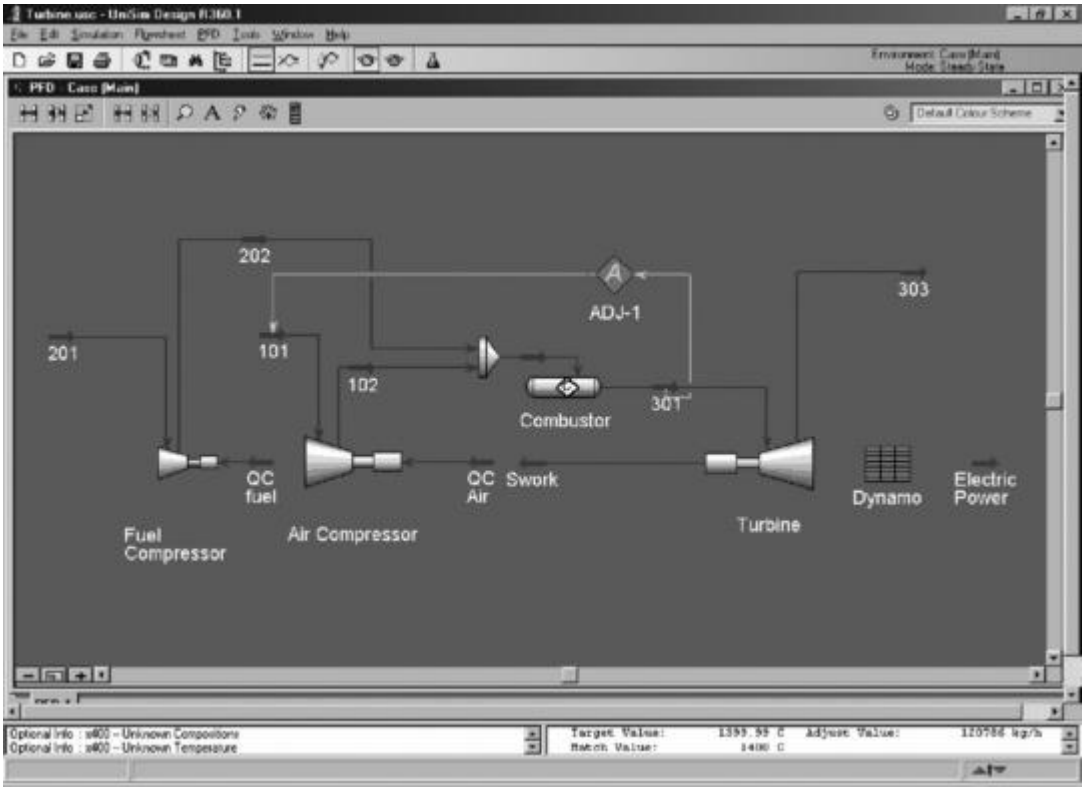


FIG. 4.33 Gas turbine model.

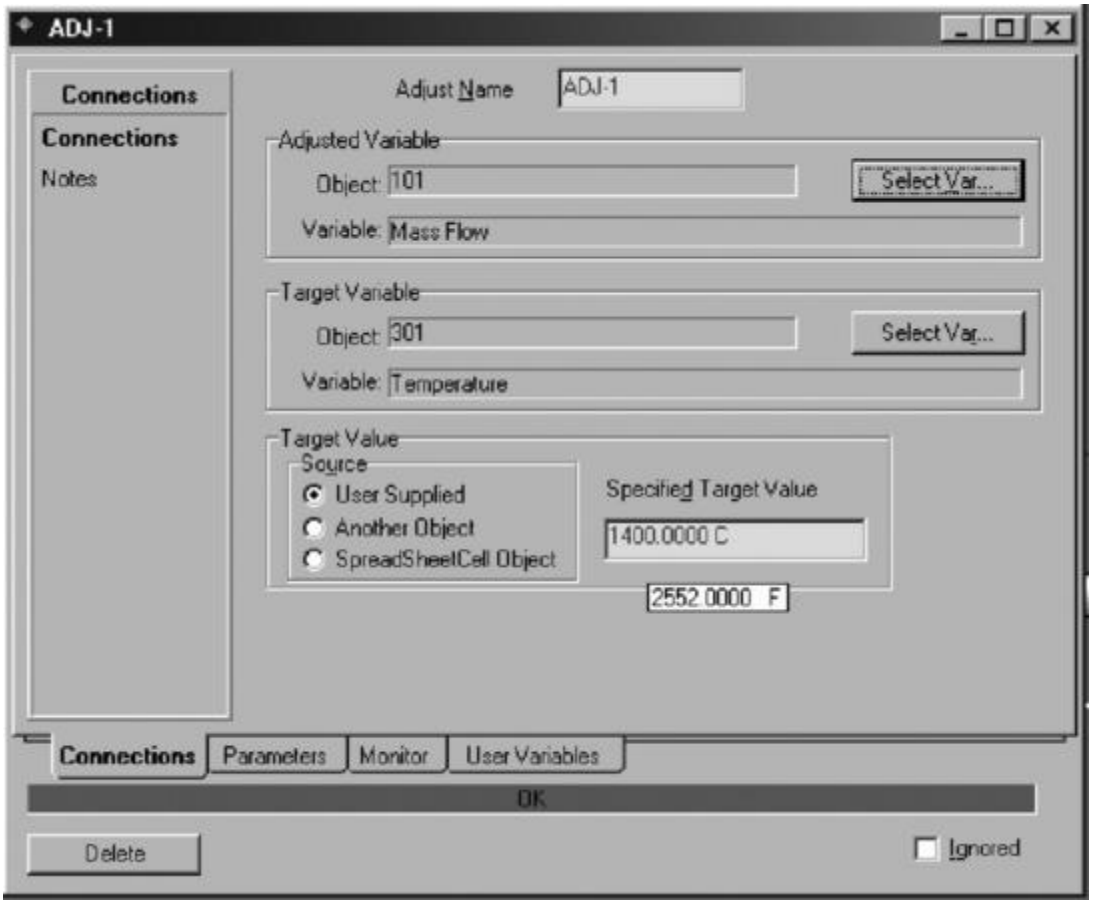


FIG. 4.34 Adjust specifications.

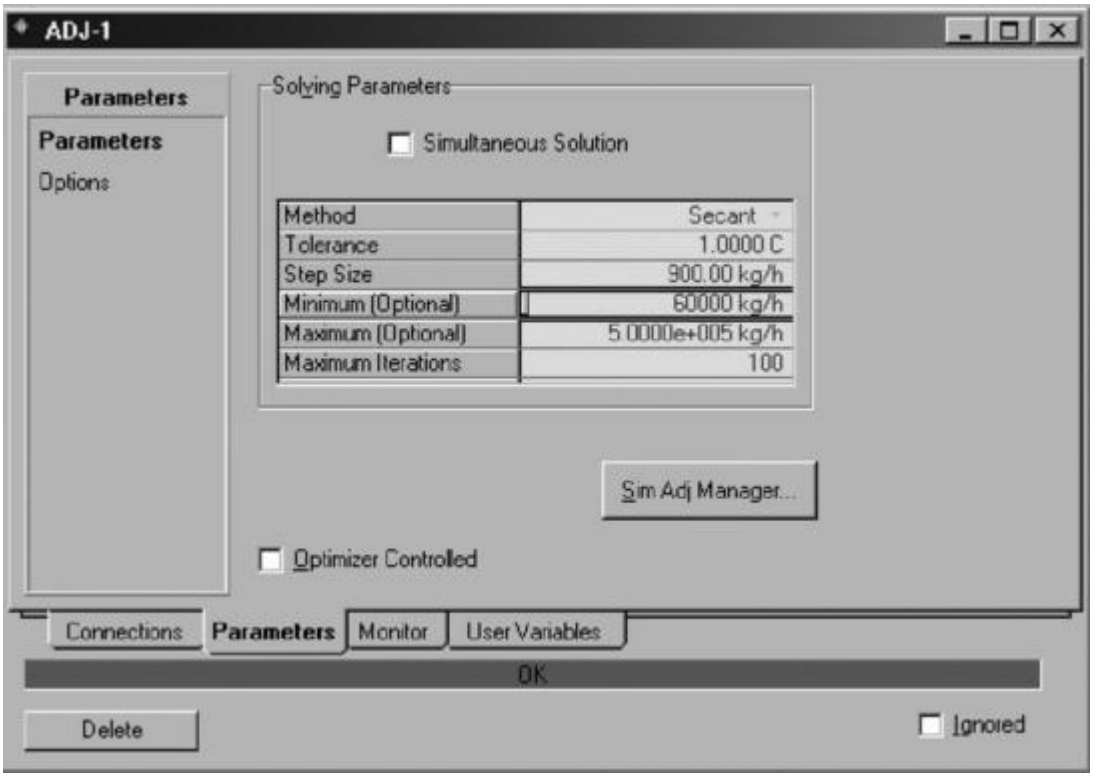


FIG. 4.35 Adjust solving parameters.

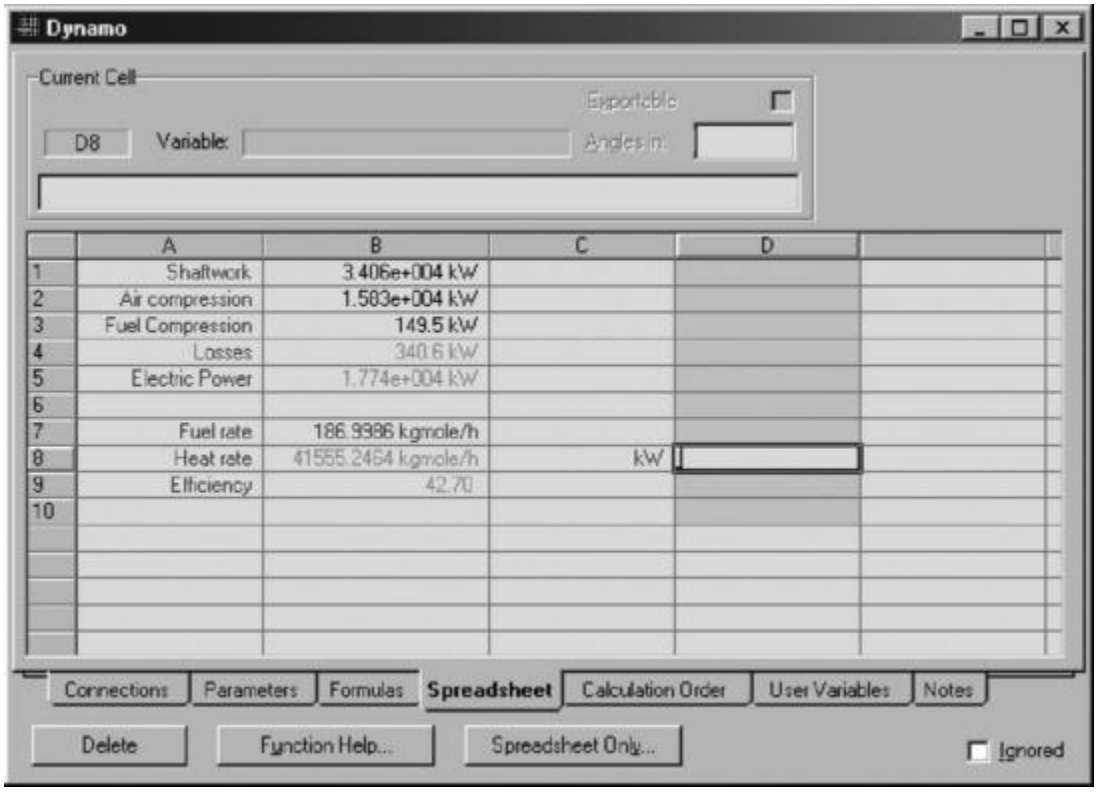


FIG. 4.36 Spreadsheet model of dynamo.

and compressor duties are then subtracted from the shaft work to give the net power from the dynamo, which is calculated to be 17.7 MW.

The cycle efficiency is the net power produced divided by the heating rate of the fuel. The heating rate is the molar flow of fuel multiplied by the standard molar heat of combustion:

$$\text{Heating rate (kW)} = \text{molar flow(mol/h)} \times \Delta H_c^{\circ}\text{(kJ/mol)}/3600 \tag{4.13}$$

The cycle efficiency is calculated to be 42.7%.

4.7 Flowsheets with recycle

Recycles of solvents, catalysts, unconverted feed materials, and by-products are found in many processes. Most processes contain at least one material recycle, and some may have six or more. Furthermore, when energy is recovered by process-to-process heat transfer, energy recycles are created, as discussed in Section 4.5.4.

4.7.1 Tearing the flowsheet

For a sequential-modular simulation program to be able to solve a flowsheet with a recycle, the design engineer needs to provide an initial estimate of a stream somewhere in the recycle loop. This is known as a *"tear" stream*, as the loop is "torn" at that point. The program can then solve and update the tear stream values with a new estimate. The procedure is repeated until the difference between values at each iteration becomes less than a specified tolerance, at which point the flowsheet is said to be converged to a solution.

The procedure for tearing and solving a simulation can be illustrated by a simple example. Fig. 4.37 shows a process in which two feeds, A and B, are combined and fed to a fixed-bed reactor. The reactor product is sent to a stripping column to remove light ends and is then sent to a column that separates heavy product from unreacted feed B. The unreacted feed B is recycled to the reactor.

To solve the reactor model, we need to specify the reactor feeds, streams 2 and 4. Stream 4 is made by adding fresh feed stream 1 to recycle stream 3, so a logical first approach might be to make an estimate of the recycle stream, in which case stream 3 is the tear stream. Fig. 4.38 shows the flowsheet torn at stream 3. The designer provides an initial estimate of stream 3a. The flowsheet then solves and calculates stream 3b. The design engineer specifies a recycle operation connecting streams 3a and 3b, and the simulator then updates stream 3a with the values from stream 3b (or with other values if an accelerated convergence method is used, as discussed later). The calculation is then repeated until the convergence criteria are met.

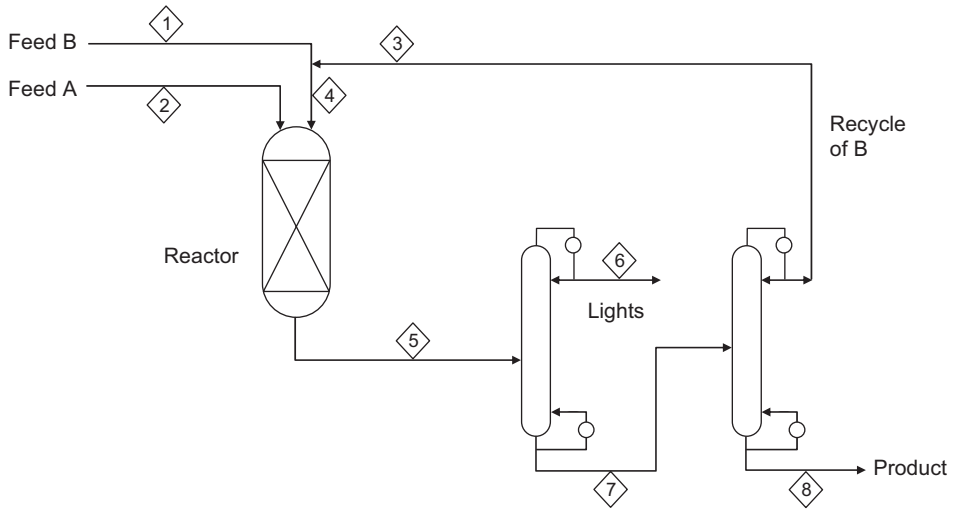


FIG. 4.37 Example process with recycle.

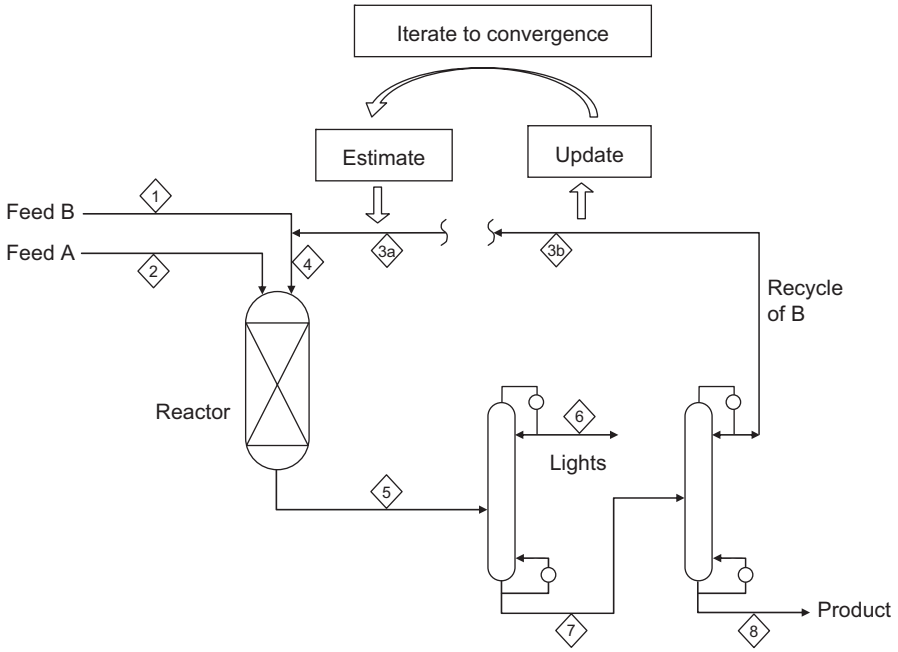


FIG. 4.38 Tearing the recycle loop.

The choice of tear stream can have a significant impact on the rate of convergence. For example, if the process in Fig. 4.37 were modeled with a yield shift reactor, then tearing the flowsheet at stream 5 would probably give faster convergence. Some of the simulation programs automatically identify the best tear stream.

4.7.2 Convergence methods

The methods used to converge recycle loops in the commercial process simulation programs are similar to the optimization methods described in Chapter 12. Most of the commercial simulation programs include the following methods.

Successive substitution (direct substitution)

In this method, an initial estimate, x_k, is used to calculate a new value of the parameter, $f(x_k)$. The estimate is then updated using the calculated value:

$$x_{k+1} = f(x_k) \tag{4.14}$$
$$x_{k+2} = f(x_{k+1}), \text{etc.}$$

This method is simple to code but is computationally inefficient and convergence is not guaranteed.

Bounded Wegstein

The bounded Wegstein method is the default method in most of the simulation programs. It is a linear extrapolation of successive substitution.

The Wegstein method initially starts out with a direct substitution step:

$$x_1 = f(x_0) \tag{4.15}$$

An acceleration parameter, q, can then be calculated:

$$q = \frac{s}{s-1} \tag{4.16}$$

$$\text{where: } s = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} \tag{4.17}$$

and the next iteration is then:

$$x_{k+1} = q\,x_k + (1-q)f(x_k) \tag{4.18}$$

If $q = 0$, the method is the same as successive substitution. If $0 < q < 1$, then convergence is damped, and the closer q is to 1.0, the slower convergence becomes. If q is less than 0, then the convergence is accelerated. The bounded Wegstein method sets bounds on q, usually keeping it in the range $-5 < q < 0$, so as to guarantee acceleration without overshooting the solution too widely.

The bounded Wegstein method is usually fast and robust. If convergence is slow, then the designer should consider reducing the bounds on q. If convergence oscillates, then consider damping the convergence by setting bounds such that $0 < q < 1$.

Newton and quasi-Newton methods

The Newton method uses an estimate of the gradient at each step to calculate the next iteration, as described in Section 12.7.4. Quasi-Newton methods such as the Broyden method use linearized secants rather than gradients. This approach reduces the number of calculations per iteration, although the number of iterations may be increased.

Newton and quasi-Newton methods are used for more difficult convergence problems, for example, when there are many recycle streams or many recycles that include operations that must be converged at each iteration, such as distillation columns. The Newton and quasi-Newton methods are also often used when there are many recycles and control blocks (see Section 4.8.1). The Newton method should not normally be used unless the other methods have failed, as it is more computationally intensive and can be slower to converge for simple problems.

4.7.3 Manual calculations

The convergence of recycle calculations is almost always better if a good initial estimate of the tear stream is provided.

If the tear stream is chosen carefully, it may be easy for the design engineer to generate a good initial estimate. This can be illustrated by returning to the problem of Fig. 4.37. We can tear the recycle loop at the reactor effluent, as shown in Fig. 4.39. We can then state the following about the reactor effluent:

1. The reactor effluent must contain the net production rate of product (which is known), plus any product that is in the recycle. Recycling product to the reactor is not a good idea, as it is likely to lead to by-product formation. A reasonable estimate of product recovery in the separation section is probably 99% or greater, so a good initial estimate of the amount of product in stream 5b is the net production rate divided by the separation recovery, or roughly 101% of the net production rate.
2. Because feed B is recycled and feed A is not, it looks like we are using an excess of B to drive full conversion of A. A good initial estimate of the flow rate of component A in stream 5b is therefore zero. If we have conversion data in terms of A, then we could produce a better estimate.
3. Feed B is supplied to the reactor in excess. The amount of B consumed in the reactor must be equal to the amount required by stoichiometry to produce the product. The amount of B remaining in the reactor effluent is given by:

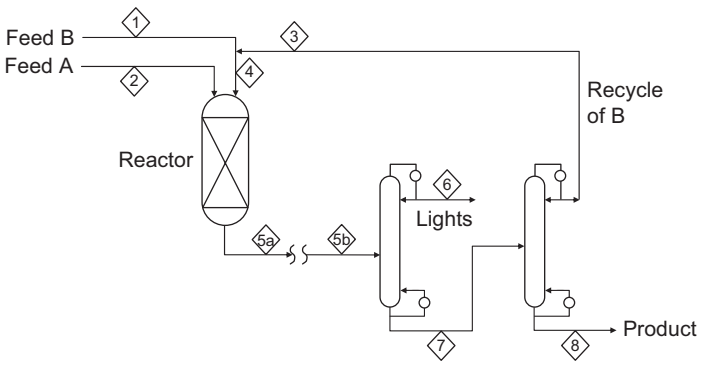


FIG. 4.39 Tearing at the reactor outlet.

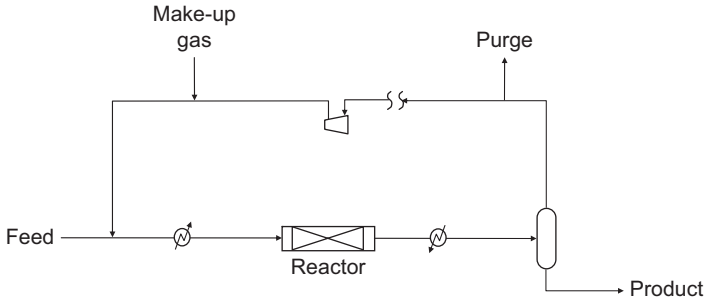


FIG. 4.40 Process with gas recycle and purge.

$$\text{moles B remaining per mole product} = \frac{\text{moles B fed}}{\text{stoichiometric moles B per mole product}} - 1$$
$$= \frac{1}{\text{conversion of B}} - 1 \tag{4.19}$$

So, knowing the flow rate of product, we can get a good initial estimate of the flow rate of B if we know either the conversion of B or the ratio in excess of the stoichiometric feed rate of B that we want to supply.

We can thus make good estimates of the three major components that are present in stream 5b. If light or heavy by-products are formed in the reactor but not recycled, then a single successive substitution step will provide good estimates for these components, as well as a better estimate of the conversion of B and the amount of A that is required in excess of stoichiometric requirements.

Manual calculations are also useful when solving flowsheets that use recycle and purge. Purge streams are often withdrawn from recycles to prevent the accumulation of species that are difficult to separate, as described in Section 2.3.4. A typical recycle and purge flow scheme is illustrated in Fig. 4.40. A liquid feed and a gas are mixed, heated, reacted, cooled, and separated to give a liquid product. Unreacted gas from the separator is recycled to the feed. A make-up stream is added to the gas recycle to make up for consumption of gas in the process. If the make-up gas contains any inert gases, over time these would accumulate in the recycle, and eventually the reaction would be slowed down when the partial pressure of reactant gas fell. To prevent this situation from occurring, we withdraw a purge stream to maintain the inerts at an acceptable level. We can provide a good initial estimate of the recycle stream by noting:

1. The flow rate of inerts in the purge is equal to the flow rate of inerts in the make-up gas.
2. The required partial pressure of reactant gas at the reactor outlet sets the concentration of reactant gas and inerts in the recycle and the unconverted gas flow rate if the reactor pressure is specified.

We can then write a mass balance on inerts:

$$F_M y_M = F_P y_R \tag{4.20}$$

and on reactant gas:

$$F_M(1-y_M) = G + F_P(1-y_R) \tag{4.21}$$

hence:

$$F_M(1-y_M) = G + F_M \frac{y_M}{y_R}(1-y_R)$$

where: F_M = make-up molar flow rate
F_P = purge molar flow rate
y_M = mole fraction of inerts in make-up
y_R = mole fraction of inerts in recycle and purge
G = molar rate of consumption of gas in reactor

Hence we can solve for M and P if G is known.

The temperature of the recycle gas at the outlet of the compressor is not easily estimated, so the logical place to tear the recycle is between the purge and the compressor, as indicated in Fig. 4.40.

4.7.4 Convergence problems

If a flowsheet is not converged, or if the process simulation software runs and gives a statement "converged with errors," then the results *cannot be used* for design. The designer must take steps to improve the simulation so that a converged solution can be found.

The first steps that an experienced designer would usually take are:

1. Make sure that the specifications are feasible.
2. Try increasing the number of iterations.
3. Try a different convergence algorithm.
4. Try to find a better initial estimate.
5. Try a different tear stream.

If one or more unit operations have been given infeasible specifications, then the flowsheet will never converge. This problem also occurs with multicomponent distillation columns, particularly when purity specifications or flow rate specifications are used or when nonadjacent key components are chosen; see Section 17.6. A quick manual mass balance around the column can usually determine whether the specifications are feasible. Remember that all the components in the feed must exit the column somewhere. The use of recovery specifications is usually more robust, but care is still needed to make sure that the reflux ratio and number of trays are greater than the minimum required. A similar problem is encountered in recycle loops if a component accumulates because of the separation specifications that have been set. Adding a purge stream usually solves this problem.

For large problems with multiple recycles, it may be necessary to increase the number of iterations to allow the flowsheet time to converge. This strategy can be effective, but is obviously inefficient if underlying problems in the model are causing the poor convergence.

In some cases, it may be worthwhile to develop a simplified simulation model to arrive at a first estimate of tear stream composition, flow rate, and conditions (temperature and pressure). Models can be simplified by using faster and more robust unit operation models, for example, substituting shortcut column models for rigorous distillation models. Models can also be simplified by reducing the number of components in the model. Reducing the number of components often leads to a good estimate of the bulk flows and stream enthalpies, which can be useful if there are interactions between the mass and energy balances. Another simplification strategy that is often used is to model heat exchangers using a dummy stream on one side (usually the side that is downstream in the process). The recycle of energy from downstream to upstream is then not converged until after the rest of the flowsheet has been converged. Alternatively, heaters and coolers can be used in a simplified model, or even in the rigorous model, as long as the stream data are then extracted and used to design the real exchangers.

Another approach that is widely used is to "creep up on" the converged solution. This entails building up the model starting from a simplified version and successively adding detail while reconverging at each step. As more complexity is added, the values from the previous run are used to initialize the next version. This is a slow but effective method. The design engineer must remember to save the intermediate versions every so often, in case later problems are encountered. A similar strategy is often used when running sensitivity analyses or case studies that require perturbations of a converged model. The designer changes the relevant parameters in small steps to reach the new conditions while reconverging at each step. The results of each step then provide a good initial estimate for the next step, and convergence problems are avoided.

When multiple recycles are present, it is sometimes more effective to solve the model in a simultaneous (equation-oriented) mode rather than in a sequential modular mode. If the simulation program allows simultaneous solution of the equation set, this can be attempted. If the process is known to contain many recycles, the designer should anticipate convergence problems and should select a process simulation program that can be run in a simultaneous mode.

Example 4.10

Light naphtha is a mixture produced by distillation of crude oil. Light naphtha primarily contains alkane compounds (paraffins), and it can be blended into gasoline. The octane value of methyl-substituted alkanes (iso-paraffins) is higher than that of straight-chain compounds (normal paraffins), so it is often advantageous to isomerize the light naphtha to increase the proportion of branched compounds.

A simple naphtha isomerization process has a feed of 10,000 barrels per day (bpd) of a 50 wt% mixture of n-hexane and methyl pentane. The feed is heated and sent to a reactor, where it is brought to equilibrium at 1300 kPa and 250 °C. The reactor

products are cooled to the dew point and fed to a distillation column operated at 300 kPa. The bottoms product of the distillation is rich in n-hexane and is recycled to the reactor feed. An overall conversion of n-hexane of 95% is achieved.

Simulate the process to determine the recycle flow rate and composition.

Solution

This problem was solved using UniSim Design. The first step is to convert the volumetric flow rate into a mass flow rate in metric units. We can set up a stream that has a 50:50 mixture by weight of n-hexane and methyl pentane. This stream has a density of 641 kg/m^3 at 40 °C, so the required flow rate is:

$$10{,}000 \text{ bpd} = 10{,}000 \times 641\left(\text{kg}/\text{m}^3\right) \times 0.1596\left(\text{m}^3/\text{bbl}\right)/24$$
$$= 42.627 \text{ metric tons/h}$$

In a real isomerization process, a part of the feed will be lost due to cracking reactions; however, in our simplified model the only reactions that occur are isomerization reactions. Because we only consider isomerization reactions, all of the product and feed components have the same molecular weight (C_6H_{14}, $M_w = 86$). The feed flow rate of n-hexane is thus $42.627 \times 0.5 = 21.31$ metric tons/h. So for 95% conversion of n-hexane, the amount of n-hexane in the product is $0.05 \times 21.31 = 1.0655$ metric tons/h, or 1065.5 / 86 = 12.39 kgmol/h. The mole fraction of n-hexane in the product is 5% of 50%, or 2.5 mol%.

To get an initial estimate of the distillation column conditions, the process was first simulated using a shortcut column model, as shown in Fig. 4.41. If we assume that no cyclic compounds are formed in the process, then the component list includes all of the available C_6 paraffin compounds (i.e., n-hexane, 2-methyl pentane, 3-methyl pentane, 2,3-methyl butane, and 2,2-methyl butane). The reactor achieves complete equilibrium between these species and so can be modeled using a Gibbs reactor.

The shortcut column model requires a second specification, given in terms of the heavy key component. We can define either of the methyl pentane species as the heavy key. In the simplified model that we have built, the level of methyl pentane in the recycle is not important to the process performance. Increasing the recycle of methyl pentane species increases the process yield of dimethyl butane species, which would lead to an improvement in the product octane number. In reality, the presence of side reactions that caused cracking to less valuable light hydrocarbons would establish a trade-off that would set the optimum level of methyl pentane recycle. For now, we will assume that the mole fraction of 2-methyl pentane in the bottoms is 0.2.

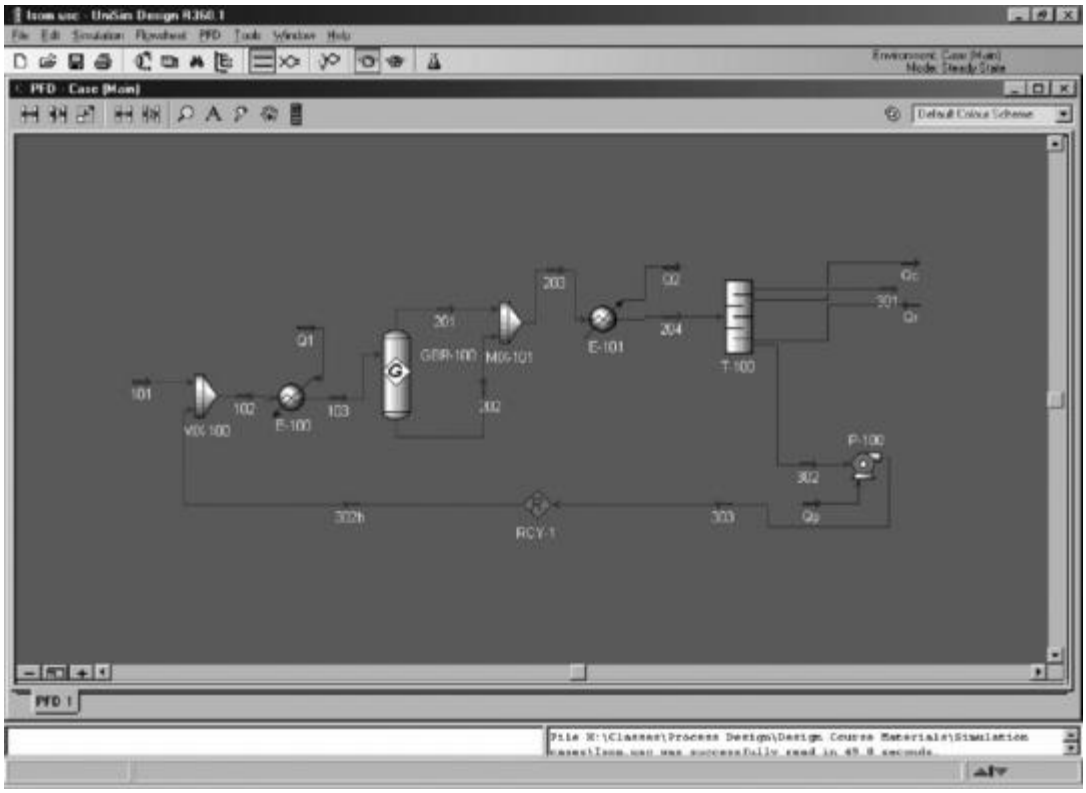


FIG. 4.41 Isomerization process model using shortcut distillation.

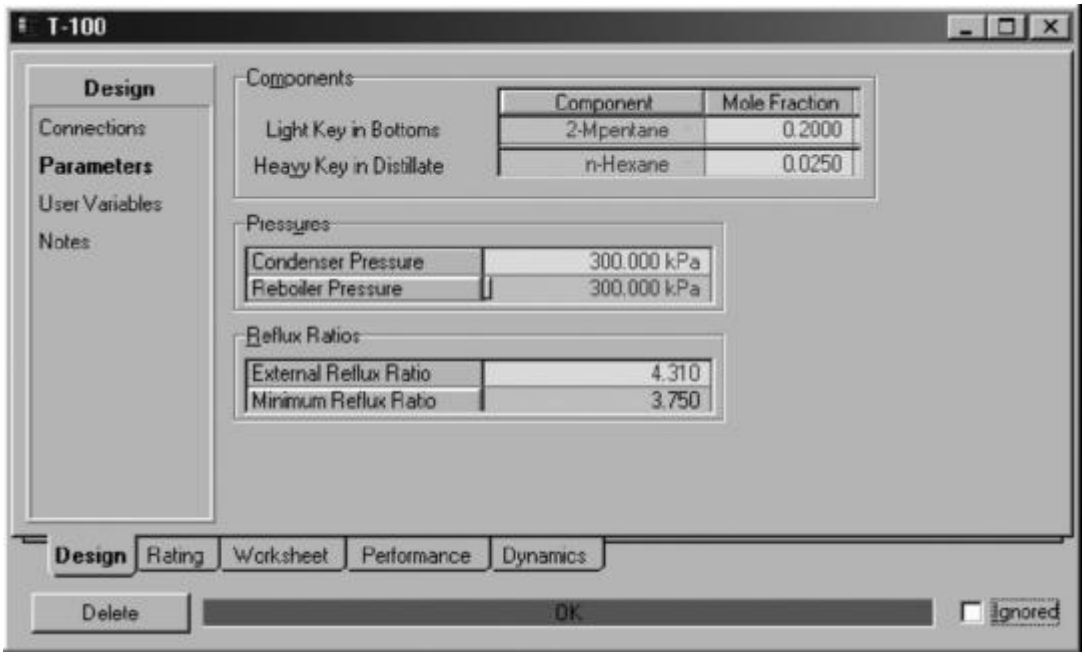


FIG. 4.42 Shortcut column specifications.

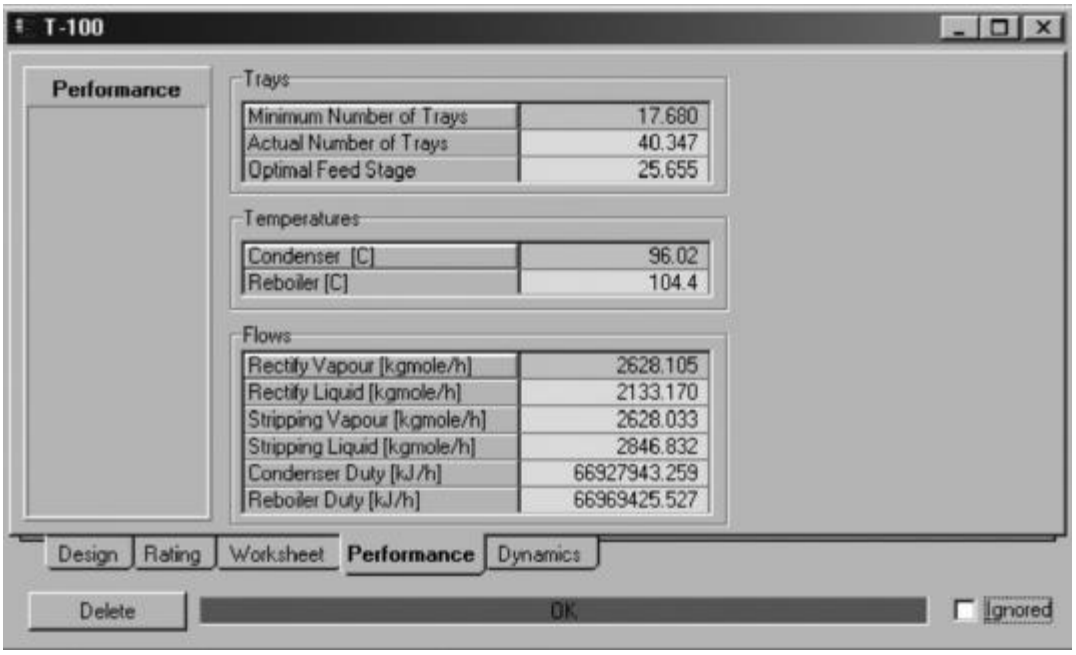


FIG. 4.43 Shortcut column results.

With these conditions, and with the recycle not closed, the shortcut column model predicts a minimum reflux of 3.75. The reflux ratio is then set at $1.15 \times R_{min} = 4.31$, as shown in Fig. 4.42. The shortcut model then calculates that we need 41 theoretical trays, with optimal feed tray 26, as shown in Fig. 4.43. The column bottoms flow rate is 18,900 kg/h, which can be used as an initial estimate for the recycle flow. The recycle loop can now be closed and run. The converged solution still has $R_{min} = 3.75$, so the reflux ratio does not need to be adjusted. The converged recycle flow rate is 18.85 metric tons/h or 218.7 kgmol/h, as shown in Fig. 4.44. The shortcut column design of the converged flowsheet still has 41 trays with the feed on tray 26.

The results from the shortcut model can now be used to provide a good initial estimate for a rigorous model. The shortcut column is replaced with a rigorous column, as shown in Fig. 4.45. The rigorous column model can be set up with the number

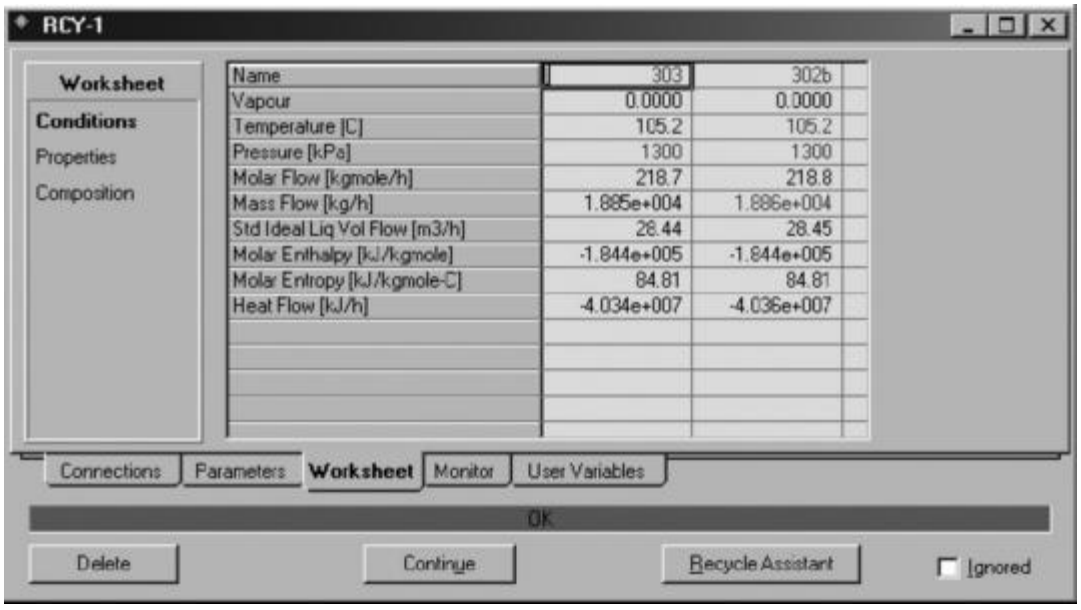


FIG. 4.44 Converged recycle results for the shortcut column model.

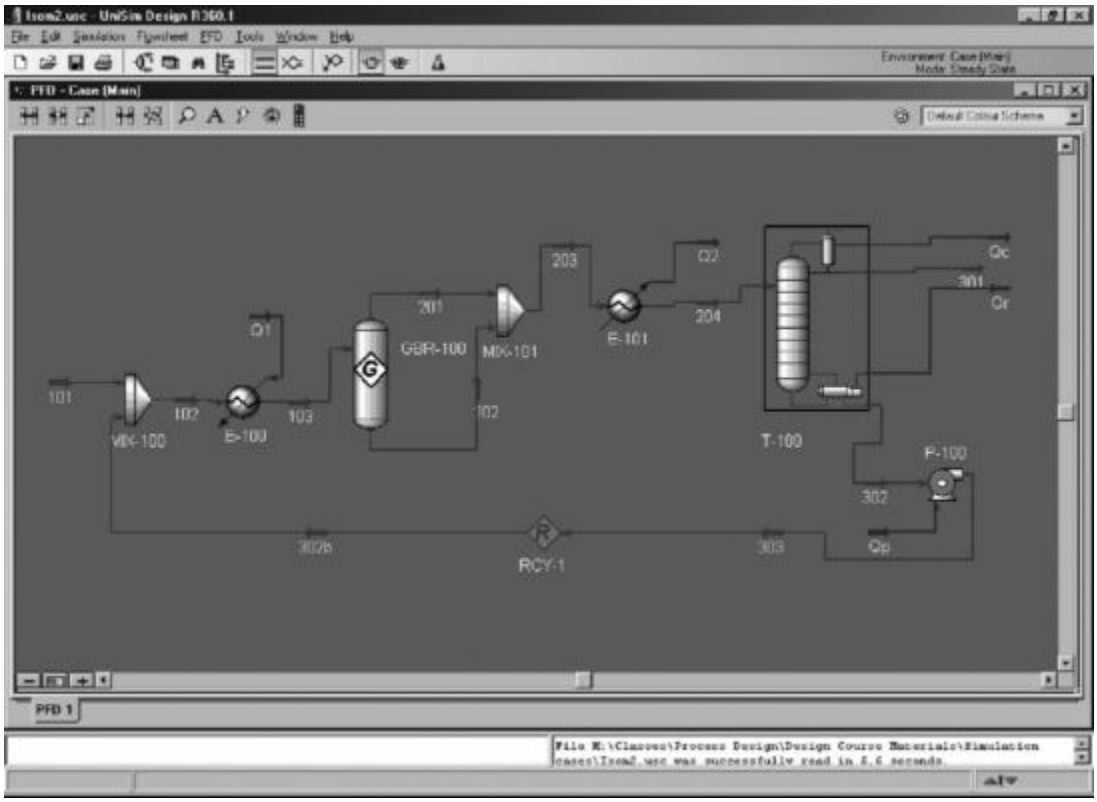


FIG. 4.45 Isomerization process model using rigorous distillation.

of stages and feed stage predicted by the shortcut model (Fig. 4.46). If we specify the reflux ratio and bottoms product rate as column specifications, as in Fig. 4.47, then the flowsheet converges quickly.

The results from the rigorous model with the inputs specified as noted earlier show a flow rate of 1084.5 kg/h of n-hexane in the distillate product. This exceeds the requirements calculated from the problem statement (1065.5 kg/h). The simplest way to get back to the required specification is to use it directly as a specification for the column. From the "Design" tab on the column window we can select "Monitor" and then "Add spec" to add a specification on the distillate flow rate of

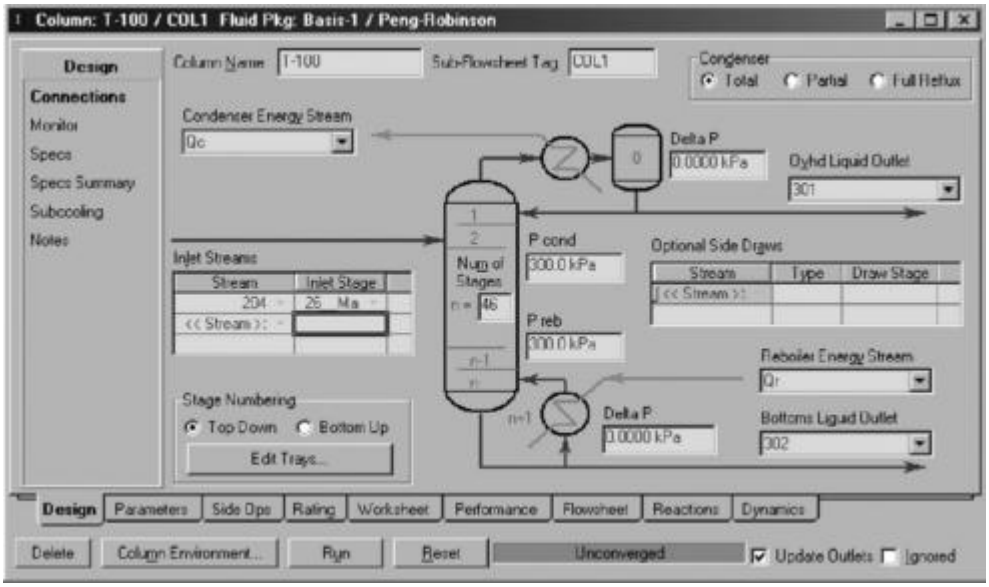


FIG. 4.46 Design parameters for the rigorous distillation column.

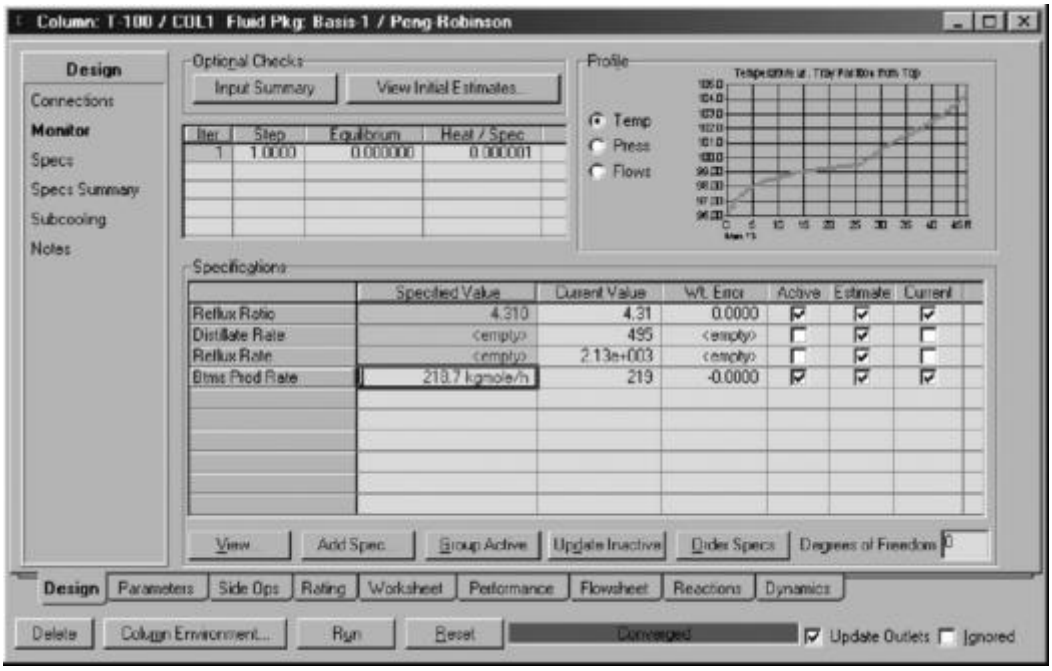


FIG. 4.47 Specifications for the rigorous distillation column.

n-hexane, as shown in Fig. 4.48. This specification can then be made active, and the bottoms flow rate specification can be relaxed. When the simulation is reconverged, the bottoms flow rate increases to 19,350 kg/h and the n-hexane in the distillate meets the specification flow rate of 1065.5 kg/h.

The column profiles for the rigorous distillation model are shown in Fig. 4.49. The profiles do not show any obvious poor design of the column, although the design is not yet optimized.

The simulation was converged to achieve the target conversion of n-hexane with a recycle of 19.35 metric tons/h. The recycle composition is 50.0 mol% n-hexane, 21.1 mol% 2-methyl pentane, 25.1 mol% 3-methyl pentane, 3.6 mol% 2,3-methyl butane, and 0.2 mol% 2,2-methyl butane. This is a converged solution, but it is only one of many possible converged solutions. No attempt has yet been made to optimize the design. The optimization of this process is examined in Problem 4.14. For more realistic information on isomerization process conditions, the reader should consult Meyers (2016).

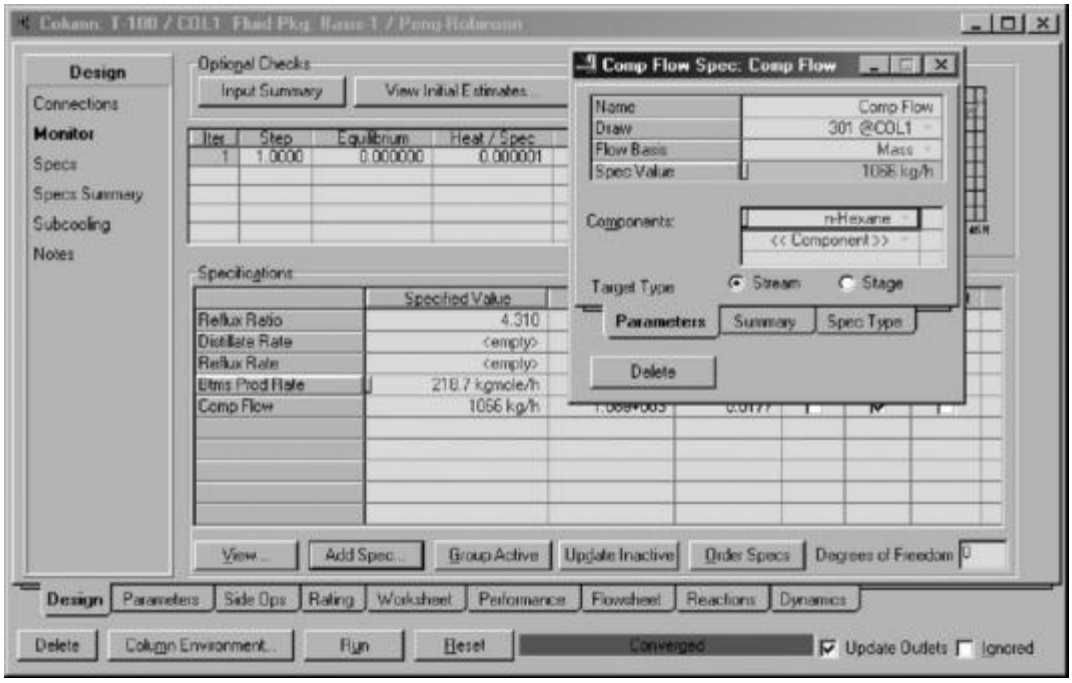


FIG. 4.48 Adding a specification on n-hexane mass flow.

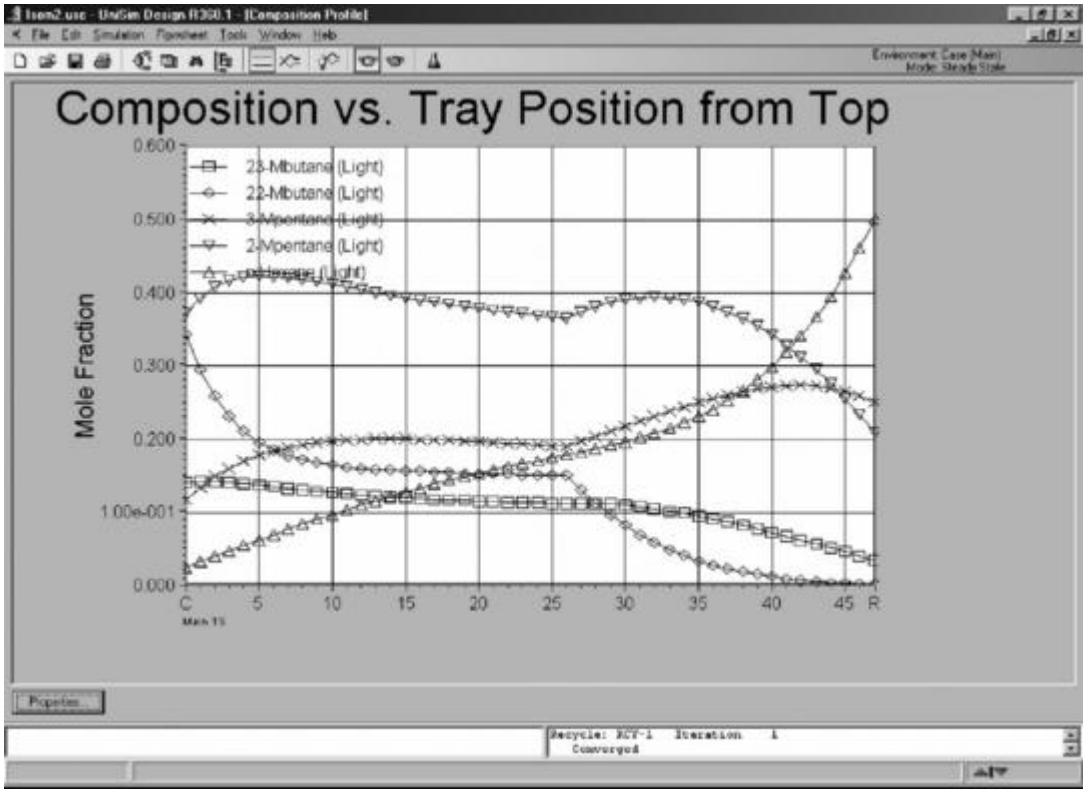


FIG. 4.49 Column profiles for the rigorous distillation model.

4.8 Flowsheet optimization

After achieving a converged simulation of the process, the designer will usually want to carry out some degree of optimization. The commercial simulation programs have a limited optimization capability that can be used with suitable caution.

4.8.1 Use of controllers

The simplest form of optimization is to impose additional constraints on the simulation so that it meets requirements specified by the designer. For example, if the designer made estimates of the feed rates, then the production rate of product that is predicted by the model may be less (or more) than the desired rate. The designer could correct this by calculating the appropriate ratio, multiplying all the feed streams by this ratio, and then reconverging the model, but this approach would soon become tedious.

Instead, the simulation programs allow the designer to impose constraints on the model. In the example noted earlier, this would be a constraint that the product flow rate is equal to a target value. Constraints are imposed using controller functions, known as a "Design Spec" in Aspen Plus or a "Set" or "Adjust" in UniSim Design. Controllers are specified either as:

$$\text{Set variable } x \text{ to value } z$$

or

$$\text{Adjust variable } x \text{ to value } y \text{ by manipulating variable } z$$

where z is an unknown variable or set of variables that will be calculated by the simulation, and x is the variable that the designer wants to specify.

Controllers can be used to capture all kinds of design constraints and specifications. They are particularly useful for setting feed ratios and controlling purge rates and recycle ratios to achieve target compositions. Some care is needed to ensure that they are used sparingly; otherwise, too many recycles of information can be introduced and convergence becomes difficult.

Controllers behave much like recycles, and it is usually a good idea to generate a converged simulation to act as a good initial estimate before adding controllers. This does not apply to simple controller functions such as feed ratio controllers.

In a dynamic simulation, controllers are used to model the real control valves of the process. When converting a steady-state simulation to a dynamic simulation, some care is needed to ensure that the controller functions correspond to physically achievable control structures.

4.8.2 Optimization using process simulation software

The commercial process simulation programs all have the ability to solve optimization problems that can be posed as nonlinear programming (NLP) problems. At the time of writing, only Aspen Plus allows the designer to carry out *discrete* optimization using integer variables. It is therefore not possible to optimize integer parameters such as feed tray location while simultaneously optimizing continuous variables in any commercial process simulation program other than Aspen Plus. Likewise, only Aspen Plus can be used to carry out superstructure optimization. Note that this discrete optimization functionality is not included in the general license of Aspen Plus, is only available in versions more recent than release 2006.5, and may not be available to all academic users. The other simulation program vendors are expected to add this capability in future releases.

Optimization of a large process simulation model is intrinsically difficult, particularly if there are multiple recycles. As noted in Section 12.10, the solution algorithms for NLP problems require multiple solutions of the model, which must be converged at each solution.

An additional complication of flowsheet optimization is the formulation of the objective function. The objective function for industrial design is always a measure of economic performance. The design parameters calculated by the simulation program can be used to give relatively good estimates of equipment cost, but this typically requires exporting the parameters into a specialized cost-estimating program, such as Aspen Icarus, as described in Section 7.10. Furthermore, the equipment must usually be oversized by a suitable design factor compared with the design flow rates, as discussed in Section 1.6. The simplest way to address this problem is to generate two or three

simulation runs with variations of the key design parameters. These designs can then be costed to develop approximate cost curves, which can then be used in the optimization tool of the simulation program.

The Aspen Plus manual provides several useful recommendations for specifying optimization problems (Aspen Technology, 2001):

1. Start by converging a simulation of the flowsheet. This helps the designer detect errors, ensures that specifications are feasible, and provides good estimates for tear streams.
2. Carry out a sensitivity analysis to determine which variables have the most impact on the objective function. These are the variables that should be used as decision variables. It is also important to determine reasonable ranges for these variables and set upper and lower bound constraints. If the ranges set are too narrow, then the optimum may not be found. If they are too wide, then convergence may be difficult.
3. While carrying out the sensitivity analysis, see if the optimum is broad or sharp. If there are only small changes in the objective function, further optimization may not be justified.

Another approach that is often used is to carry out optimization using simplified models to fix the process structure and determine the approximate values of key decision variables. A final NLP optimization can then be carried out using a rigorous model.

4.9 Dynamic simulation

Most continuous processes are only simulated in steady-state mode. Some of the simulation programs allow a steady-state simulation to be converted to run in a dynamic mode. Dynamic simulation is useful for:

1. Simulating batch and semicontinuous processes to determine rate-controlling steps and investigate batch-to-batch recycles and heat recovery
2. Simulating process start-up and shut-down
3. Simulating cyclic processes
4. Simulating process disturbances to evaluate control system performance and tune controllers
5. Simulating emergency conditions to evaluate alarm system and relief system responses and ensure that they are adequate

For a good dynamic simulation, the designer must specify the actual control system from the piping and instrumentation diagram (see Chapter 5) and also all of the vessel designs so that hold-ups can be calculated. Mass transfer rates and reaction rates must also be known or assumed.

Dynamic simulation is more computationally intensive than steady-state simulation. Dynamic simulation is usually applied to parts of a process (or even single unit operations) rather than an entire process. Different simulation strategies are needed to give a robust dynamic model. Good introductions to dynamic simulation are given in the books by Luyben (2013), Ingham et al. (2007), Seborg et al. (2016), and Asprey and Machietto (2003) and the paper by Pantelides (1988).

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4.11 Nomenclature

		Dimensions in MLT θ
A	Heat exchanger area	$\mathbf{L^2}$
A	Coefficient in the Antoine equation	—
B	Coefficient in the Antoine equation	θ
C	Coefficient in the Antoine equation	θ
C_p	Specific heat capacity at constant pressure	$\mathbf{L^2T^{-2}}\theta^{-1}$
F	Shell and tube exchanger factor (for noncountercurrent flow)	—
F_M	Make-up gas molar flow rate	$\mathbf{MT^{-1}}$
F_P	Purge gas molar flow rate	$\mathbf{MT^{-1}}$
f_i	Fugacity coefficient for component i	—
f_i^{OL}	Standard state fugacity coefficient of pure liquid	—
G	Molar rate of consumption of gas in reactor	$\mathbf{MT^{-1}}$
K	Equilibrium constant (ratio)	—
L_v	Latent heat of vaporization	$\mathbf{L^2T^{-2}}$
$L_{v,b}$	Latent heat at normal boiling point	$\mathbf{L^2T^{-2}}$
M	Molecular mass (weight)	$\mathbf{M}$
P	Pressure	$\mathbf{ML^{-1}T^{-2}}$
P_c	Critical pressure	$\mathbf{ML^{-1}T^{-2}}$
P_i^0	Vapor pressure of component i	$\mathbf{ML^{-1}T^{-2}}$ or $\mathbf{L}$
P_r	Reduced pressure	—
ΔP_c	Critical constant increment in Lydersen equation (Equation 4.5)	$\mathbf{M^{-1/2}L^{1/2}T}$
q	Wegstein method acceleration parameter	—
s	Wegstein method estimate of gradient	—
T	Temperature, absolute scale	θ
T_c	Critical temperature	θ
T_r	Reduced temperature	θ
ΔT_c	Critical constant increment in Lydersen equation (Equation 4.4)	—
U	Overall heat transfer coefficient	$\mathbf{MT^{-3}}\theta^{-1}$
ΔV_c	Critical constant increment in Lydersen equation (Equation 4.6)	$\mathbf{M^{-1}L^3}$
v_i^L	Liquid molar volume	$\mathbf{M^{-1}L^3}$
x	Mol fraction, liquid phase	—
x	Controlled parameter	—
x_k	Estimate of parameter x at kth iteration	—
y	Target value	—
y	Mol fraction, vapor phase	—
y_M	Mole fraction of inerts in make-up	—
y_R	Mole fraction of inerts in recycle and purge	—
z	Target value or unknown variable calculated by simulation program	—
z	Compressibility factor	—
γ	Liquid activity coefficient	—
ϕ	Fugacity coefficient	—
ϕ^s	Fugacity coefficient of pure component	—
Suffixes		
a, b i, j, k 1, 2	Components	—
L	Liquid	—
V	Vapor	—

4.12 Problems

4.1. Monochlorobenzene is produced by the reaction of benzene with chlorine. A mixture of monochlorobenzene and dichlorobenzene is produced, with a small amount of trichlorobenzene. Hydrogen chloride is produced as a by-product. Benzene is fed to the reactor in excess to promote the production of monochlorobenzene.

The reactor products are fed to a condenser, where the chlorobenzenes and unreacted benzene are condensed. The condensate is separated from the noncondensable gases in a separator. The noncondensables—hydrogen chloride and unreacted chlorine—pass to an absorption column where the hydrogen chloride is absorbed in water. The chlorine leaving the absorber is recycled to the reactor.

The liquid phase from the separator, containing chlorobenzenes and unreacted benzene, is fed to a distillation column, where the chlorobenzenes are separated from the unreacted benzene. The benzene is recycled to the reactor.

Using the data given here, calculate the stream flows and draw up a preliminary flowsheet for the production of 1.0 ton (metric ton) of monochlorobenzene per day.
Data:

Reactor

$$\text{Reactions: } C_6H_6 + Cl_2 \rightarrow C_6H5 + HCl$$
$$C_6H_6 + 2Cl_2 \rightarrow C_6H_4Cl_2 + 2HCl$$

mol ratio $Cl_2 : C_6H_6$ at inlet to reactor = 0.9
overall conversion of benzene = 55.3%
yield of monochlorobenzene = 73.6%
yield of dichlorobenzene = 27.3%
Production of other chlorinated compounds can be neglected.

Separator

Assume 0.5% of the liquid stream is entrained with the vapor.

Absorber

Assume 99.99% absorption of hydrogen chloride and that 98% of the chlorine is recycled, with the remainder being dissolved in the water. The water supply to the absorber is set to produce a 30% w/w strength hydrochloric acid.

Distillation column

Take the recovery of benzene to be 95% and 99.99% recovery of the chlorobenzenes.

Note:
This problem can be solved without using process simulation software. Start the mass balance at the reactor inlet (after the recycle streams have been added) and assume 100 kgmol/h of benzene at this point.

4.2. Methyl tertiary butyl ether (MTBE) is used as an antiknock additive in gasoline. It is manufactured by the reaction of isobutene with methanol. The reaction is highly selective, and practically any C_4 stream containing isobutene can be used as a feedstock

$$CH_2 = C(CH_3)_2 + CH_3OH \rightarrow (CH3)3 - C - O - CH_3$$

A 10% excess of methanol is used to suppress side reactions.
In a typical process, the conversion of isobutene in the reactor stage is 97%.
The product is separated from the unreacted methanol and any C_4 compounds by distillation.

The essentially pure, liquid MTBE leaves the base of the distillation column and is sent to storage. The methanol and C_4 compounds leave the top of the column as vapor and pass to a column where the methanol is separated by absorption in water. The C_4 compounds leave the top of the absorption column, saturated with water, and are used as a fuel gas. The methanol is separated from the water solvent by distillation and recycled to the reactor stage. The water, which leaves the base of the column, is recycled to the absorption column. A purge is taken from the water recycle stream to prevent the buildup of impurities.

1. Draw up a block flow diagram for this process.
2. Estimate the feeds for each stage.
3. Draw a flowsheet for the process.

Treat the C_4 compounds other than isobutene as one component.
Data:

1. Feedstock composition, mol%: n-butane = 2, butene-1 = 31, butene-2 = 18, isobutene = 49.
2. Required production rate of MTBE, 7000 kg/h.
3. Reactor conversion of isobutene, 97%.
4. Recovery of MTBE from the distillation column, 99.5%.
5. Recovery of methanol in the absorption column, 99%.
6. Concentration of methanol in the solution leaving the absorption column, 15%.
7. Purge from the water recycle stream to waste treatment, 10% of the flow leaving the methanol recovery column.
8. The gases leave the top of the absorption column saturated with water at 30 °C.
9. Both columns operate at essentially atmospheric pressure.

4.3. Ethanol can be produced by fermentation of sugars and is used as a gasoline blending component. Because the sugars can be derived from biomass, ethanol is potentially a renewable fuel. In the fermentation of cane sugar to ethanol, sucrose ($C_{11}H_{22}O_{11}$) is converted by yeast (*Saccharomyces cerevisiae*) to yield ethanol and CO_2. Some sucrose is also consumed in maintaining the cell culture in the fermentation reactor. The fermentation reaction can be carried out in a continuous reactor as long as the ethanol concentration does not exceed about 8 wt%, at which point the productivity of the yeast declines significantly. The sucrose is fed as a 12.5 wt% solution in water, which must be sterilized before it can be fed to the reactor. The sterilization is usually accomplished by heating with steam. Carbon dioxide is vented from the fermentation reactor. The liquid product of the fermentation reactor is sent to a hydrocyclone to concentrate the yeast for recycle to the reactor. The remaining liquid is sent to a distillation column known as a *beer column*, which concentrates the alcohol to about 40 mol% ethanol and 60 mol% water in the distillate. The recovery of ethanol in the beer column is 99.9%. The bottoms stream from the beer column contains the remaining components of the fermentation broth and can be processed for use as animal feed.

1. Draw a flowsheet for this process.
2. Estimate the stream flow rates and compositions for a production rate of 200,000 U.S. gal/d of dry (100%) ethanol.
3. Estimate the ethanol lost in the CO_2 vent gas.
4. Estimate the reboiler duty of the beer column.

Data:

1. Yield per kg sucrose: ethanol 443.3 g, CO_2 484 g, nonsugar solids 5.3 g, yeast 21 g, fermentation by-products 43.7 g, higher alcohols (fusel oil) 2.6 g.
2. Conversion of sucrose, 98.5%.
3. Yeast concentration in fermentation reactor at steady state, 3 wt%.
4. Fermenter temperature, 38 °C.

4.4. In an ethanol plant, the mixture of water and ethanol from the beer column distillate contains about 40% ethanol (molar basis) in water, together with the fusel oils described in the previous problem. This mixture is distilled to give an azeotropic mixture of ethanol and water (89% ethanol) overhead, with 99.9% recovery of ethanol. The fusel oil can cause blending problems if it is allowed to accumulate in the distillate. Fusel oil is a mixture of higher alcohols and ethers that can be approximated as a mixture of n-butanol and diethyl ether. This mixture is usually removed as a side stream from the column. When the side stream is contacted with additional water a two-phase mixture can be formed, and the oil phase can be decanted to leave an ethanol–water phase that is returned to the column.

1. Draw a flowsheet for this process.
2. Estimate the stream flow rates and compositions for a production rate of 200,000 U.S. gal/d of dry (100%) ethanol.
3. Optimize the distillation column using the cost correlations given in Section 6.3 and assuming that reboiler heat costs $5/MMBtu. Minimize the total annualized cost of the column.

4.5. Water and ethanol form a low-boiling-point azeotrope; hence water cannot be completely separated from ethanol by conventional distillation. To produce absolute (100%) ethanol, it is necessary to add an entraining agent to break the azeotrope. Benzene is an effective entrainer and is used where the product is not required for food products. Three columns are used in the benzene process.

Column 1. This column separates the ethanol from the water. The bottom product is essentially pure ethanol. The water in the feed is carried overhead as the ternary azeotrope of ethanol, benzene, and water (roughly 24% ethanol, 54% benzene, 22% water). The overhead vapor is condensed and the condensate separated in a decanter into a benzene-rich phase (22% ethanol, 74% benzene, 4% water) and a water-rich phase (35% ethanol, 4% benzene, 61% water). The benzene-rich phase is recycled to the column as reflux. A benzene make-up stream is added to the reflux to make up any loss of benzene from the process. The water-rich phase is fed to the second column.

Column 2. This column recovers the benzene as the ternary azeotrope and recycles it as vapor to join the overhead vapor from the first column. The bottom product from the column is essentially free of benzene (29% ethanol, 51% water). This stream is fed to the third column.

Column 3. In this column, the water is separated and sent to waste treatment. The overhead product consists of the azeotropic mixture of ethanol and water (89% ethanol, 11% water). The overheads are condensed and recycled to join the feed to the first column. The bottom product is essentially free of ethanol.

1. Draw a flowsheet for this process.
2. Estimate the stream flow rates and compositions for a production rate of 200,000 U.S. gal/d of dry (100%) ethanol.
3. Estimate the ethanol lost in the CO_2 vent gas.

Take the benzene losses to total 0.1 kmol/h. All the compositions given are molar percentages.

4.6. A plant is required to produce 10,000 tons per year of anhydrous hydrogen chloride from chlorine and hydrogen. The hydrogen source is impure: 90 mol% hydrogen, balance nitrogen. The chlorine is essentially pure chlorine, supplied in rail tankers.

The hydrogen and chlorine are reacted in a burner at 1.5 bar pressure.

$$H_2 + Cl_2 \rightarrow 2HCl$$

Hydrogen is supplied to the burner in 3% excess over the stoichiometric amount. The conversion of chlorine is essentially 100%. The gases leaving the burner are cooled in a heat exchanger.

The cooled gases pass to an absorption column, where the hydrogen chloride gas is absorbed in dilute hydrochloric acid. The absorption column is designed to recover 99.5% of the hydrogen chloride in the feed.

The unreacted hydrogen and inerts pass from the absorber to a vent scrubber, where any hydrogen chloride present is neutralized by contact with a dilute, aqueous solution of sodium hydroxide. The solution is recirculated around the scrubber. The concentration of sodium hydroxide is maintained at 5% by taking a purge from the recycle loop and introducing a make-up stream of 25% concentration. The maximum concentration of hydrogen chloride discharged in the gases vented from the scrubber to atmosphere must not exceed 200 ppm (parts per million) by volume.

The strong acid from the absorption column (32% HCl) is fed to a stripping column, where the hydrogen chloride gas is recovered from the solution by distillation. The diluted acid from the base of this column (22% HCl) is recycled to the absorption column.

The gases from the top of the stripping column pass through a partial condenser, where the bulk of the water vapor present is condensed and returned to the column as reflux. The gases leaving the column will be saturated with water vapor at 40 °C.

The hydrogen chloride gas leaving the condenser is dried by contact with concentrated sulfuric acid in a packed column. The acid is recirculated over the packing. The concentration of sulfuric acid is maintained at 70% by taking a purge from the recycle loop and introducing a make-up stream of strong acid (98% H_2SO_4).

The anhydrous hydrogen chloride product is compressed to 5 bar and supplied as a feed to another process.

Using the information provided, calculate the flow rates and compositions of the main process streams, and draw a flowsheet for this process. All compositions are wt%, except where indicated.

4.7. Ammonia is synthesized from hydrogen and nitrogen. The synthesis gas is usually produced from hydrocarbons. The most common raw materials are oil or natural gas, though coal and even peat can be used.

When produced from natural gas, the synthesis gas will be impure, containing up to 5% inerts, mainly methane and argon. The reaction equilibrium and rate are favored by high pressure. The conversion is low, about 15%, and so after removal of the ammonia produced, the gas is recycled to the converter inlet. A typical process consists of a converter (reactor) operating at 350 bar, a refrigerated system to condense out the ammonia product from the recycle loop, and compressors to compress the feed and recycle gas. A purge is taken from the recycle loop to keep the inert concentration in the recycle gas at an acceptable level.

Using the data given here, draw a flow diagram of the process and calculate the process stream flow rates and compositions for the production of 600 t/d ammonia.

Data:

Composition of synthesis gas, mol fraction:

N_2	H_2	CH_4	A
24.5	73.5	1.7	0.3

Temperature and operating pressure of liquid ammonia–gas separator, 340 bar and −28 °C.
Inert gas concentration in recycle gas, not greater than 15 mol%.

4.8. Methyl ethyl ketone (MEK) is manufactured by the dehydrogenation of 2-butanol.

A simplified description of the process listing the various units used is given here:

1. A reactor in which the butanol is dehydrated to produce MEK and hydrogen, according to the reaction:

$$CH_3CH_2CH_3CHOH \rightarrow CH_3CH_2CH_3CO + H_2$$

The conversion of alcohol is 88%, and the selectivity to MEK can be taken as 100%.

2. A cooler-condenser, in which the reactor off-gases are cooled and most of the MEK and unreacted alcohol are condensed. Two exchangers are used, but they can be modeled as one unit. Of the MEK entering the unit, 84% is condensed, together with 92% of the alcohol. The hydrogen is noncondensable. The condensate is fed forward to the final purification column.
3. An absorption column in which the uncondensed MEK and alcohol are absorbed in water. Around 98% of the MEK and alcohol can be considered to be absorbed in this unit, giving a 10 wt% solution of MEK. The water feed to the absorber is recycled from the next unit, the extractor. The vent stream from the absorber, containing mainly hydrogen, is sent to a flare stack.
4. An extraction column in which the MEK and alcohol in the solution from the absorber are extracted into trichloroethane (TCE). The raffinate, water containing around 0.5 wt% MEK, is recycled to the absorption column.

   The extract, which contains around 20 wt% MEK, and a small amount of butanol and water, is fed to a distillation column.
5. A distillation column that separates the MEK and alcohol from the solvent TCE. The recovery of MEK is 99.99%.

   The solvent containing a trace of MEK and water is recycled to the extraction column.
6. A second distillation column that produces a 99.9% pure MEK product from the crude product from the first column. The residue from this column, which contains the bulk of the unreacted 2-butanol, is recycled to the reactor.

For a production rate of 1250 kg/h MEK:

1. Draw a flowsheet for the process.
2. Estimate the stream flow rates and compositions.
3. Estimate the reboiler and condenser duties of the two distillation columns.
4. Estimate the number of theoretical trays required in each column.

4.9. In the problem of Example 4.4, the feed was specified as pentane (C_5H_{12}) with a hydrogen-to-carbon ratio of 2.4:1. If the feed to the process were a heavy oil, the hydrogen-to-carbon ratio would be more like 2:1. How would the distribution of C_5 carbon compounds change if the feed had a 2:1 carbon ratio?

4.10. Example 4.4 examined the equilibrium distribution of hydrocarbon compounds within a single carbon number (C_5). In reality, cracking reactions to ethylene, propylene, and other light alkenes and alkynes will have a significant effect on the yield of a cracking process.

1. What is the effect of including C_2 and C_3 compounds on the equilibrium distribution?
2. What is the effect of including coke (carbon) as well as the C_2 and C_3 compounds?
3. What do these results tell you about cracking processes?

4.11. Optimize the heat exchanger design of Example 4.8 to minimize the total surface area required.

4.12. A stream containing 4 metric tons/h of a 20 wt% mixture of benzene in toluene is heated from 20 °C to the bubble point at 4 atm pressure. The mixture is separated in a distillation column to give 99.9% recovery of benzene overhead and toluene in the bottoms.

1. If the toluene product must be cooled to 20 °C, how much of the feed heat can be supplied by heat exchange with the bottoms?
2. How many heat exchange shells are needed?
3. What is the minimum total heat exchange area?
4. What is the distillation column diameter?
5. How many sieve trays are needed if the tray efficiency is 70%?

4.13. The autothermal reforming of methane to hydrogen was described in Example 4.5. The solution in the example was not optimized, and suggestions were given for how to improve the results. Optimize the process to minimize the cost of production of hydrogen, assuming:

1. Cost of methane = 16 ¢/lb
2. Cost of oxygen = 2 ¢/lb
3. Cost of water = 25 ¢/1000 lb
4. Annualized cost of heat exchangers = \$ 30,000 + 3 A, where A is the area in ft^2
5. Cost of electric power = 6 ¢/kWh
6. Reactor and catalyst costs are the same in all cases.

Hint: First determine the optimal heat recovery and steam and oxygen to methane ratios for a given methane conversion. Repeat for different methane conversions to find the overall optimum.

4.14. The light naphtha isomerization process is more complex than the description given in Example 4.10.

1. Hydrogen is flowed through the plant to reduce catalyst deactivation. The hydrogen flow rate is typically about 2 moles per mole of hydrocarbon on a pure hydrogen basis. The hydrogen make-up gas is typically about 90 mol% hydrogen, with the balance comprising methane.
2. Light hydrocarbon compounds are formed by cracking reactions. These compounds accumulate in the hydrogen recycle and are controlled by taking a purge stream. A stabilizer column is also required, upstream of the distillation column, to remove light hydrocarbons and hydrogen before the distillation.
3. Each of the C_6 isomers has a different blending octane value. The total octane value of the product can be found by summing the products of the mole fraction of each component and the component blending value. The blending values are n-hexane 60; 2-methyl pentane 78.5; 3-methyl pentane 79.5; 2,2-dinethyl butane 86.3; and 2,3-dimethyl butane 93.

Optimize the design of Example 4.10, subject to the following:

1. The selectivity loss due to cracking reactions can be approximated as 1% conversion of C_6 compounds to propane per reactor pass.
2. The wholesale value of gasoline can be assumed to be 2.0 + 0.05 (octane number − 87) $/US gal.
3. The cost of hydrogen is $6/1000 scf, and the fuel value of the hydrogen and propane purge stream is $5/MMBtu.
4. The reactor plus catalyst total installed cost can be taken as $0.5 MM per 1000 bpd of liquids processed.
5. Other costs can be estimated using the cost correlations given in Table 7.2.

4.15 The composition of the feed to a debutanizer is given here. The column will operate at 14 bar and below 750 K. The process is to be modeled using a commercial simulation program. Suggest a suitable phase equilibrium method to use in the simulation.

Feed composition:

		kg/h
Propane	C3	910
Isobutane	i-C4	180
n-butane	n-C4	270
Isopentane	i-C5	70
normal pentane	n-C5	90
normal hexane	n-C6	20

4.16. The product specifications for Problem 4.15 are 99.5% recovery of C_5+ in the bottoms and 99% recovery of C_4 and lighter compounds in the distillate. Your company's corporate engineering standard is to design for a reflux ratio of 1.15 times the minimum reflux and to assume a stage efficiency of 60%. Using rigorous simulation, determine the number of trays, feed tray, and reboiler duty for this column.

4.17. In the manufacture of methyl ethyl ketone from butanol, the product is separated from unreacted butanol by distillation. The feed to the column consists of a mixture of methyl ethyl ketone, 2-butanol, and trichloroethane. What would be a suitable phase equilibrium correlation to use in modeling this process?

Additional flowsheeting problems are given in the form of design projects in Appendices E and F. Additional reaction and distillation simulation problems are given in Chapters 15 and 17, respectively.

CHAPTER

5

Instrumentation and process control

KEY LEARNING OBJECTIVES

- How to read a piping and instrument diagram drawn using ANSI/ISA 5.1 symbols
- How to design control schemes for common unit operations and whole processes

5.1 Introduction

The process flowsheet shows the arrangement of the major pieces of equipment and their interconnection. It is a description of the nature of the process.

The piping and instrument diagram (P&I diagram or PID) shows the engineering details of the equipment, instruments, piping, valves and fittings, and their arrangement. It is often called the *engineering flowsheet* or *engineering line diagram*. This chapter covers the preparation of the preliminary P&I diagrams at the process design stage of the project.

Some process control information is also indicated on the process flow diagram (PFD). It is common practice to show control valves on the PFD but to omit isolation valves, relief valves, and instrumentation details. Control valves require a significant pressure drop to operate effectively, so the location of control valves will often indicate a need for additional pumps or compressors. In some cases, process control considerations may even lead to the addition of vessels to the flowsheet; for instance, when a surge tank is added to smooth out operation between batch and continuous sections of the plant.

The design of piping systems, and the specification of the process instrumentation and control systems, is usually done by specialist design groups, and a detailed discussion of control systems is beyond the scope of this book. Only general guide rules are given. The piping handbook edited by Nayyar (2000) and the process automation handbook by Love (2007) are particularly recommended for guidance on the detailed design of piping systems and process instrumentation and control. The references cited in the text and listed at the end of the chapter should also be consulted. The detailed design of piping systems, valves, and plant hydraulics and the sizing and selection of control valves are discussed in more detail in Chapter 20.

5.2 The P&I diagram

The P&I diagram shows the arrangement of the process equipment, piping, pumps, instruments, valves, and other fittings. It should include:

1. All process equipment identified by an equipment number. The equipment should be drawn roughly in proportion, and the location of nozzles shown.

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2. All pipes identified by a line number. The pipe size and material of construction should be shown. The material may be included as part of the line identification number.
3. All valves—control and block valves—with an identification number. The type and size should be shown. The type may be shown by the symbol used for the valve or included in the code used for the valve number.
4. Ancillary fittings that are part of the piping system, such as inline sight-glasses, strainers, and steam traps, with an identification number.
5. Pumps identified by a suitable code number.
6. All control loops and instruments with an identification number.

For simple processes, the utility (service) lines can be shown on the P&I diagram. For complex processes, separate diagrams should be used to show the service lines so the information can be shown clearly, without cluttering up the diagram. The service connections to each unit should, however, be shown on the P&I diagram.

The P&I diagram will resemble the process flowsheet, but the process information is not shown. The same equipment identification numbers should be used on both diagrams.

5.2.1 Symbols and layout

The symbols used to show the equipment, valves, instruments, and control loops will depend on the practice of the particular design office. The equipment symbols are usually more detailed than those used for the process flowsheet. A typical example of a P&I diagram is shown in Fig. 5.22 at the end of this chapter.

The most widely used international standard symbols for instruments, controllers, and valves are those given by the Instrumentation Systems and Automation Society design code ANSI/ISA 5.1-2009. Some companies use their own symbols, though, and different standards are followed in some countries, such as BS 1646 in the United Kingdom and DIN 19227 and DIN 2429 (now both superseded by DIN 28000-4) in Germany.

When laying out the diagram, it is only necessary to show the relative elevation of the process connections to the equipment where these affect the process operation; for example, the net positive suction head (NPSH) of pumps, barometric legs, siphons, and the operation of thermosiphon reboilers. Full details of pipe layout are usually shown in a different drawing, known as a *piping isometric drawing*. See Fig. 20.21 for an example.

Computer-aided drafting programs are available for the preparation of P&I diagrams. Microsoft Visio Professional edition contains a library of P&I diagram symbols.

5.2.2 Basic symbols

The symbols illustrated in Figs. 5.1 to 5.7 are those given in ANSI/ISA 5.1-2009.

Control valves

Different types of valves are shown in Fig. 5.1 and discussed in Section 20.5.

Actuators

Actuator symbols are illustrated in Fig. 5.2.

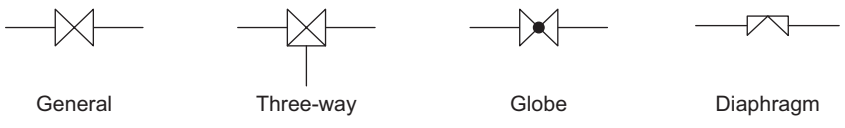


FIG. 5.1 Control valves.

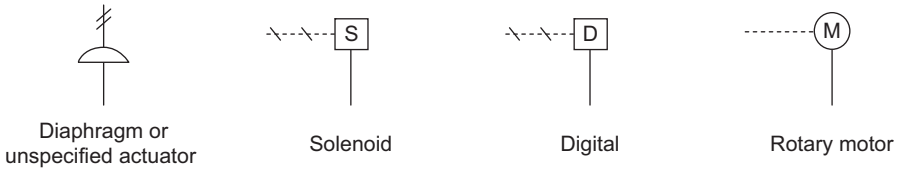


FIG. 5.2 Actuators.

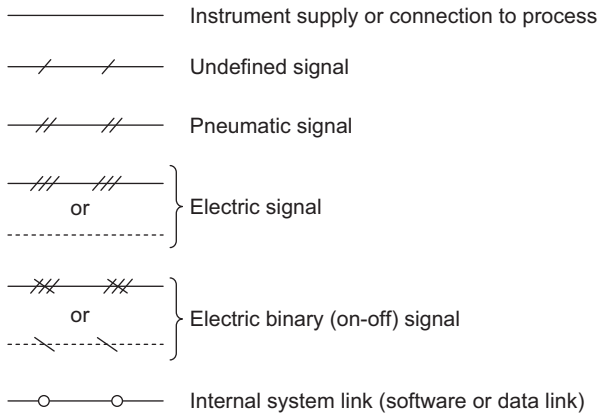


FIG. 5.3 Instrument lines.

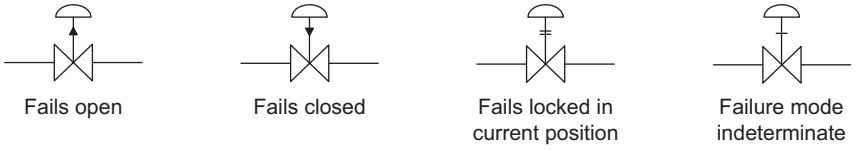


FIG. 5.4 Valve failure modes.

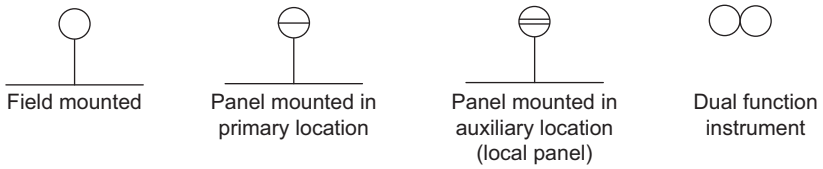


FIG. 5.5 General instrument and controller symbols.

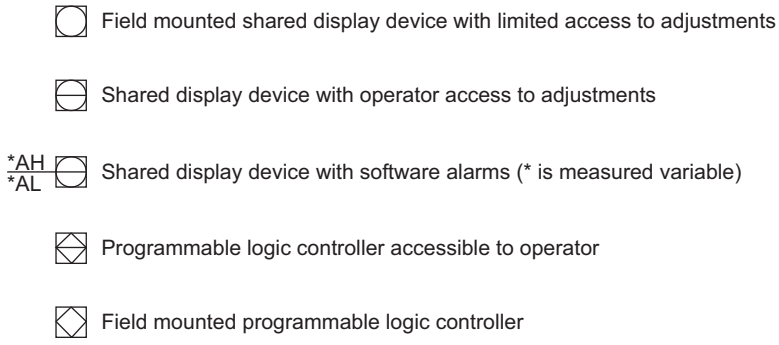


FIG. 5.6 Shared display symbols for distributed control and logic control.

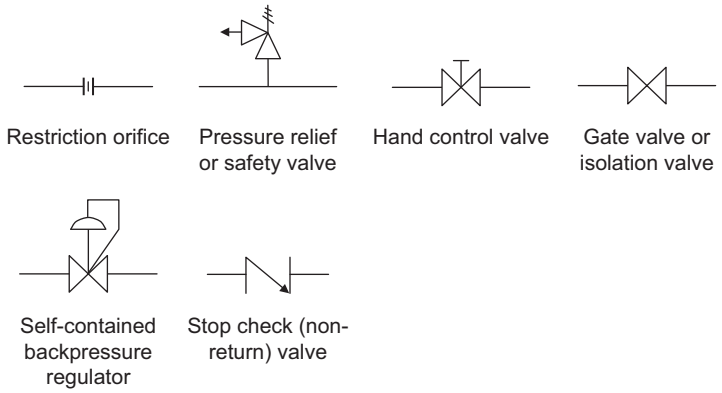


FIG. 5.7 Other common symbols.

Most modern control valves (final control elements) are actuated by electric motors, but older valves are actuated by pneumatic signals using instrument air. Pneumatic actuators are preferred in situations where electronic controllers might cause a process hazard or where electric power is not available or reliable. Pneumatic controllers are also found in many older plants where replacement with electronic controllers has not yet occurred. Motor actuators are used for larger valves, and digital and solenoid actuators are used for valves that switch from open to closed, as often occurs in batch processing. Many newer controllers use a combination of these approaches. For example, a digital signal can be sent to a solenoid that opens or shuts an instrument air line that then actuates a pneumatically driven control valve.

Instrument Lines

The instrument connecting lines are drawn in a manner to distinguish them from the main process lines, as shown in Fig. 5.3. Process lines are drawn as solid lines and are usually drawn thicker. The undefined signal symbol is often used when indicating controllers in a PFD, as the instrument design may not have been specified when the PFD was first drawn.

Failure mode

The direction of the arrow shows the position of the valve on failure of the power supply (Fig. 5.4).

General instrument and controller symbols

General instrument symbols are shown in Fig. 5.5.

Locally mounted means that the controller and display are located out on the plant near the sensing instrument location. *Main panel* means that they are located on a panel in the control room. Except on small plants, most controllers would be mounted in the control room.

Distributed control: Shared display symbols

Symbols for shared displays and programmable logic controllers are shown in Fig. 5.6.

A distributed control system is a system that is functionally integrated but consists of subsystems that may be physically separate and remotely located from one another. A shared display is an operator interface device such as a computer screen or video screen that is used to display process control information from a number of sources at the command of the operator. Most plants built since 1990 (and many older plants) use shared displays instead of instrument panels.

Programmable logic controllers are used to control discrete operations, such as steps in a batch or semicontinuous process, and to program interlock controls that guard against unsafe or uneconomic conditions. For example, a logic controller could be used to ensure that an operator cannot open an air vent line to a vessel unless the feed valves are closed and nitrogen purge is open.

Other common symbols

Other symbols commonly encountered on a P&I diagram are shown in Fig. 5.7.

Type of instrument

This is indicated on the circle representing the instrument controller by a letter code (Table 5.1).

TABLE 5.1 Letter code for instrument symbols (based on ISA-5.1-1984 [R1992])

Initiating or measured variable	First letter	Indicating only	Controllers			Transmitters	Final control element
			Recording	Indicating	Blind		
Analysis (composition)	A	AI	ARC	AIC	AC	AT	AV
Flow rate	F	FI	FRC	FIC	FC	FT	FV
Flow ratio	FF	FFI	FFRC	FFIC	FFC	FFT	FFV
Power	J	JI	JRC	JIC		JT	JV
Level	L	LI	LRC	LIC	LC	LT	LV
Pressure, vacuum	P	PI	PRC	PIC	PC	PT	PV
Pressure differential	PD	PDI	PDRC	PDIC	PDC	PDT	PDV
Quantity	Q	QI	QRC	QIC		QT	QZ
Radiation	R	RI	RRC	RIC	RC	RT	RZ
Temperature	T	TI	TRC	TIC	TC	TT	TV
Temperature differential	TD	TDI	TDRC	TDIC	TDC	TDT	TDV
Weight	W	WI	WRC	WIC	WC	WT	WZ

Notes:
1. The letters C, D, G, M, N, and O are not defined and can be used for any user-specified property.
2. The letter S as second or subsequent letter indicates a switch.
3. The letter Y as second or subsequent letter indicates a relay or a compute function.
4. The letter Z is used for the final control element when this is not a valve.
Consult the standard for the full set of letter codes.

The first letter indicates the property measured; for example, F = flow. Subsequent letters indicate the function; for example,

$$\text{I} = \text{indicating}$$

$$\text{RC} = \text{recorder controller}$$

The letters AH or AL indicate high or low alarms, respectively.

The P&I diagram shows all the components that make up a control loop. For example, Fig. 5.8 shows a field located pressure transmitter connected to a shared display pressure indicator-controller with operator access to adjustments and high and low alarms. The pressure controller sends an electric signal to a fail-closed diaphragm-actuated pressure control valve.

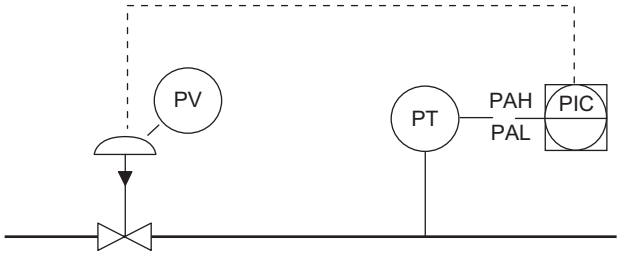


FIG. 5.8 A typical control loop.

5.3 Process instrumentation and control

5.3.1 Instruments

Instruments are provided to monitor the key process variables during plant operation. They may be incorporated in automatic control loops or used for manual monitoring of process operation. In most modern plants, the instruments will be connected to a computer control and data logging system. Instruments monitoring critical process variables will be fitted with automatic alarms to alert the operators to critical and hazardous situations.

Details of process instruments and control equipment can be found in various handbooks: Green and Southard (2018), Love (2007), and Liptak (2012). Reviews of process instruments and control equipment are published periodically in the journals *Chemical Engineering* and *Hydrocarbon Processing*. These reviews give details of instruments and control hardware available commercially. Table 5.2 summarizes some of the more commonly used types of instruments encountered in chemical plants.

TABLE 5.2 Commonly used process instruments

Measured variable	Instrument type	Operating principle
Pressure (gauge)	Differential pressure (DP) cell	Pressure difference causes displacement of a diaphragm. The displacement can be transmitted mechanically to a bellows to register a pneumatic signal or converted to an electrical signal by a strain gauge or by movement of the diaphragm relative to a static capacitor plate. Gauge pressure is measured relative to atmospheric pressure.
Pressure difference	DP cell	As earlier. Pressure difference is measured between two points in the process.
Temperature	Thermocouple	Wires of different metals joined together to form a circuit with one joint hotter than the other will develop an EMF through the Seebeck effect. If one joint is at a reference temperature, the other temperature can be found from the EMF. The reference temperature is usually ambient temperature, which is determined by measuring the electrical resistance of a platinum wire. Different combinations of metal wire are used depending on the temperature range. See Love (2007) for details of thermocouple types.
Volumetric flow	Orifice meter	Flow passes through a restriction orifice. Pressure difference across the orifice is measured with a DP cell. Flow rate is calculated from pressure drop.
Volumetric flow	Venturi meter	Flow passes through a shaped pipe restriction. Pressure difference across the restriction is measured with a DP cell. Flow rate is calculated from pressure drop.
Mass flow	Coriolis meter	Flow through a shaped vibrating pipe loop causes it to twist due to the Coriolis effect. The extent of twist is measured optically. These instruments can be used for multiphase flow, but are expensive, particularly for large flow rates.

TABLE 5.2 Commonly used process instruments—cont'd

Measured variable	Instrument type	Operating principle
Level	DP cell	A DP cell placed between the top and bottom of a vessel can indicate level if there is no internal pressure drop in the vessel.
Level	Capacitance probe	The capacitance between a probe in the center of the vessel and the wall is affected by the dielectric constant of the material between them, and so varies with level.
Interface level	DP cell	A DP cell can determine the interface level between immiscible fluids if they are in a vessel that has an internal weir (so that overall level remains constant).
pH	Glass electrode	The glass electrode and a reference electrode (usually silver/silver chloride) form an electrochemical circuit allowing EMF to be measured.
Composition	Chromatograph	Gas chromatography (GC) can be used to separate simple mixtures and generate a signal through a thermal conductivity detector (TCD) or flame ionization detector (FID). GC methods are difficult to use for online control because the chromatography typically takes a few minutes, but they can be used in cascade control schemes to adjust set points on other controllers.

The process variable that is to be monitored should be measured directly; however, this is often impractical, and some dependent variable that is easier to measure is monitored in its place. For example, in the control of distillation columns, the continuous, online analysis of the overhead product is desirable but is difficult and expensive to achieve reliably, so temperature is often monitored as an indication of composition. The temperature instrument may form part of a control loop controlling, say, reflux flow, with the composition of the overheads checked frequently by automated sampling and online gas chromatograph (GC) analysis.

5.3.2 Instrumentation and control objectives

The primary objectives of the designer when specifying instrumentation and control schemes are:

1. Safe plant operation:
   - **a.** To keep the process variables within known safe operating limits.
   - **b.** To detect dangerous situations as they develop and to provide alarms and automatic shut-down systems.
   - **c.** To provide interlocks and alarms to prevent dangerous operating procedures.
2. Production rate:
   - **a.** To achieve the design product output.
3. Product quality:
   - **a.** To maintain the product composition within the specified quality standards.
4. Cost:
   - **a.** To operate at the lowest production cost, commensurate with the other objectives.
5. Stability:
   - **a.** To maintain steady, automatic plant operation with minimal operator intervention.

These are not separate objectives and must be considered together. The order in which they are listed is not meant to imply the precedence of any objective over another, other than that of putting safety first. Product quality, production rate, and the cost of production will be dependent on sales requirements. For example, it may be a better strategy to produce a better-quality product at a higher cost.

In a typical chemical processing plant these objectives are achieved by a combination of automatic control, manual monitoring, and laboratory and online analysis.

5.3.3 Automatic control schemes

The detailed design and specification of the automatic control schemes for a large project are usually done by specialists. The basic theory underlying the design and specification of automatic control systems is covered in several texts: Coughanowr and LeBlanc (1994), Shinskey (1984, 1996), Luyben et al. (1999), Henson et al. (1996), Seborg et al. (2017), Love (2007), Chhabra and Rohani (2017), and Green and Southard (2018). The books by Murrill (1988), Shinskey (1996), Kalani (2002), and Love (2007) cover many of the more practical aspects of process control system design and are recommended.

In this chapter only the first step in the specification of the control systems for a process will be considered: the preparation of a preliminary scheme of instrumentation and control, developed from the process flowsheet. This can be drawn up by the process designer based on experience with similar plants and critical assessment of the process requirements. Many of the control loops will be conventional, and a detailed analysis of the system behavior will not be needed, nor justified. Judgment, based on experience, must be used to decide which systems are critical and need detailed analysis and design.

Some examples of typical (conventional) control systems used for the control of specific process variables and unit operations are given in the next section and can be used as a guide in preparing preliminary instrumentation and control schemes.

Guide rules

The following procedure can be used when drawing up preliminary P&I diagrams:

1. Identify and draw in those control loops that are obviously needed for steady plant operation, such as:
   - **a.** Level controls
   - **b.** Flow controls
   - **c.** Pressure controls
   - **d.** Temperature controls
2. Identify the key process variables that need to be controlled to achieve the specified product quality. Include control loops using direct measurement of the controlled variable, where possible; if not practicable, select a suitable dependent variable.
3. Identify and include those additional control loops required for safe operation not already covered in steps 1 and 2.
4. Decide and show those ancillary instruments needed for the monitoring of the plant operation by the operators and for troubleshooting and plant development. It is well worth including additional connections for instruments that may be needed for future troubleshooting and development, even if the instruments are not installed permanently. These would include extra thermowells, pressure taps, orifice flanges, and sample points.
5. Decide on the location of sample points.
6. Decide on the type of control instrument that will be used, including whether it will be a local instrument or tied into the plant computer control system. Also decide on the type of actuator that can be used, the signal system, and whether the instrument will record data. This step should be done in conjunction with steps 1 to 4.
7. Decide on the alarms and interlocks needed; this should be done in conjunction with step 3 (see Chapter 10).

In step 1 it is important to remember the following basic rules of process control:

There can only be a single control valve on any given stream between unit operations.
A level controller is needed anywhere where a vapor–liquid or liquid–liquid interface is maintained.
Pressure control is more responsive when the pressure controller actuates a control valve on a vapor stream.
Two operations cannot be controlled at different pressures unless there is a valve or other restriction (or a compressor or pump) between them.

Temperature control is usually achieved by controlling the flow of a utility stream (such as steam or cooling water) or a bypass around an exchanger.
The overall plant material balance is usually set by flow controllers or flow ratio controllers on the process feeds. There cannot be an additional flow controller on an intermediate stream unless there is provision for accumulation (surge), such as an intermediate storage tank.

Some simple examples of control schemes for common unit operations are given in the next section.

5.4 Conventional control schemes

5.4.1 Level control

In any equipment where an interface exists between two phases (e.g., a liquid and a vapor), some means of maintaining the interface at the required level must be provided. This may be incorporated in the design of the equipment, for example, by providing an internal weir, or by automatic control of the flow from the equipment. Fig. 5.9 shows a typical arrangement for the level control at the base of a column. The control valve should be placed on the discharge line from the pump.

5.4.2 Pressure control

Pressure control will be necessary for most systems handling vapor or gas. The method of control depends on the nature of the process. Typical schemes are shown in Figs. 5.10(a)–(d). The scheme shown in Fig. 5.10(a) would not be used where the vented gas was toxic or valuable. In these circumstances the vent should be taken to a vent recovery system, such as a scrubber. The controls shown in Fig. 5.10(b)–(d) are commonly used for controlling the pressure of distillation columns.

In processes that have a high-pressure reaction section and low-pressure separation section, the high-pressure section is usually pressure controlled by expanding the product from the high-pressure section across a control valve. If the process fluid does not change phase, then a more economical scheme is to expand the product through a turbine or turbo-expander and recover shaft work from the expansion.

5.4.3 Flow control

Flow control is usually associated with inventory control in a storage tank or other equipment or with feeds to the process. There must be a reservoir upstream of the control valve to take up the changes in flow rate.

To provide flow control on a compressor or pump running at a fixed speed and supplying a near-constant volume output, a bypass control would be used, as shown in Fig. 5.11(a). The use of variable-speed motors, as shown in

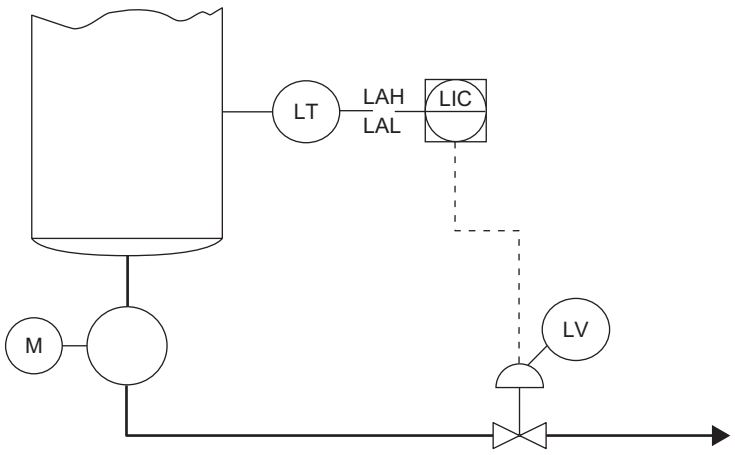


FIG. 5.9 Level control.

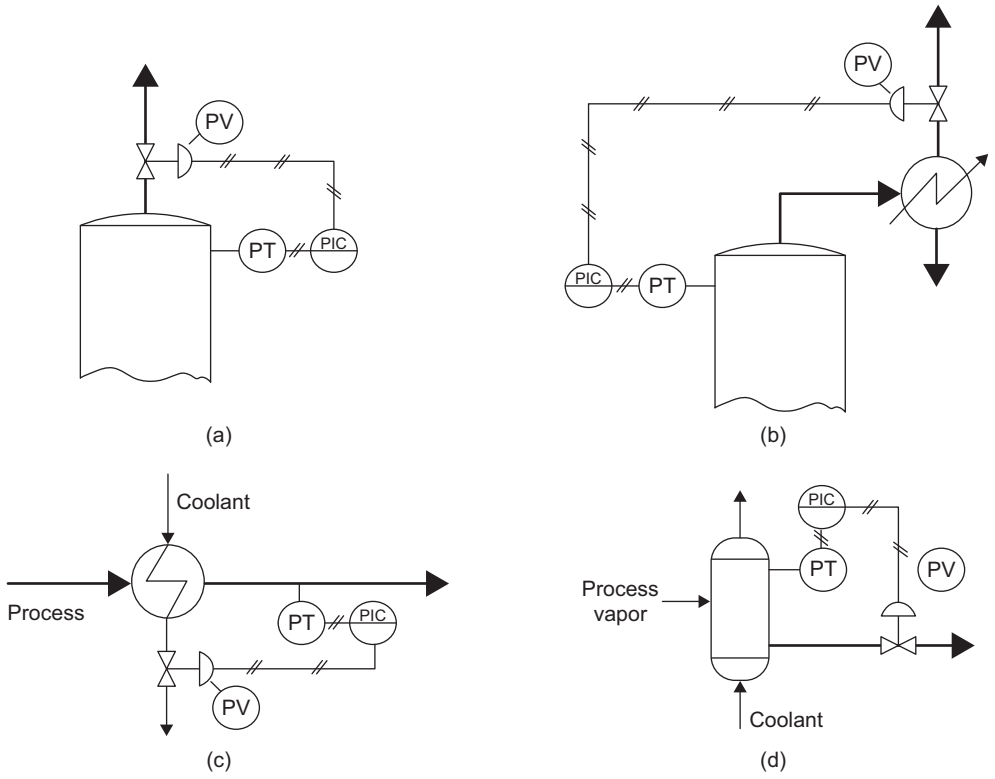


FIG. 5.10 (a) Pressure control by direct venting. (b) Venting of noncondensibles after a condenser. (c) Condenser pressure control by controlling coolant flow. (d) Pressure control of a condenser by varying the heat-transfer area, with the area dependent on liquid level.

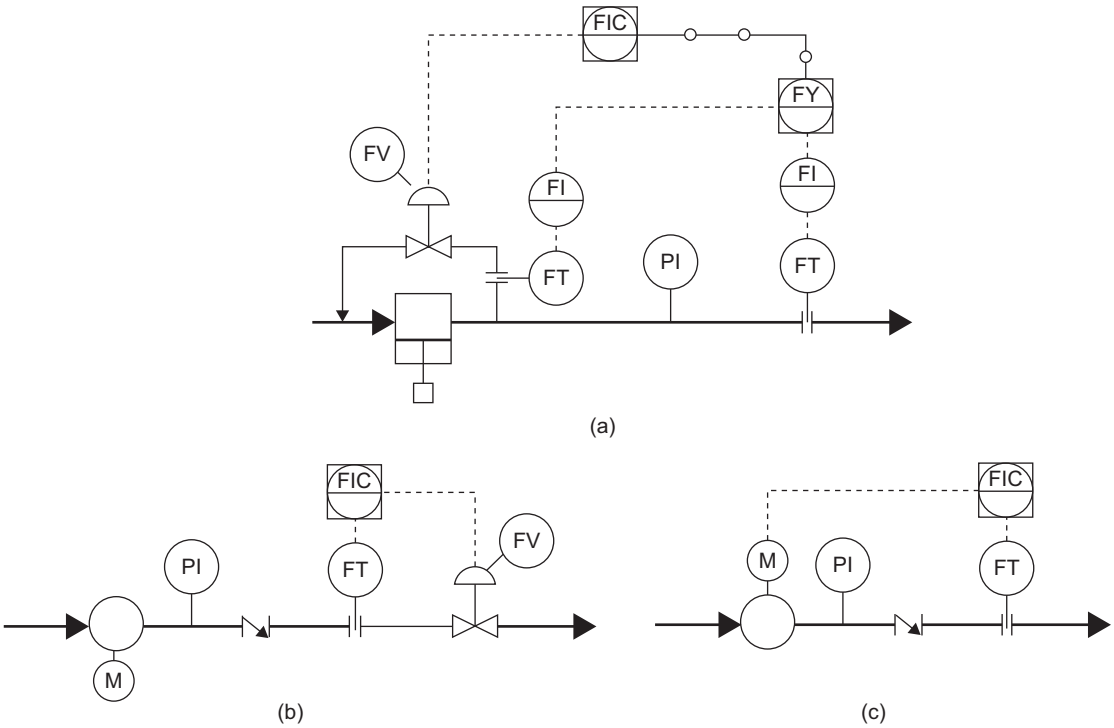


FIG. 5.11 (a) Spill-back flow control for a reciprocating pump. (b) Flow control for a centrifugal pump. (c) Centrifugal pump with variable-speed drive.

Fig. 5.11(c), is more energy efficient than the traditional arrangement shown in Fig. 5.11(b) and is becoming increasingly common; see Hall (2010).

The overall process material balance is usually set by flow controllers on the feed streams. These will often control feeds in ratio to a flow of valuable feed, a solid stream flow (which is difficult to change quickly), or a measured flow of process mixture. Flow rates of small streams are often controlled using special metering pumps that deliver a constant mass flow rate.

The design of pump and control valve systems to assure a desired process flow rate and range of controllability is discussed in more detail in Chapter 20.

5.4.4 Heat exchangers

Fig. 5.12(a) shows the simplest arrangement: the temperature being controlled by varying the flow of the cooling or heating medium.

If the exchange is between two process streams whose flows are fixed, bypass control will have to be used, as shown in Fig. 5.12(b).

For air coolers, the coolant temperature may vary widely on a seasonal (or even hourly) basis. A bypass on the process side can be used, as shown in Fig. 5.12(c), or else a variable-speed motor can be used, as shown in Fig. 5.12(d).

Condenser control

Temperature control is unlikely to be effective for condensers, unless the liquid stream is subcooled. Pressure control is often used, as shown in Fig. 5.10(d), or control can be based on the outlet coolant temperature. Condenser control is discussed in more detail by Kister (2016).

Reboiler and vaporizer control

As with condensers, temperature control is not effective, as the saturated vapor temperature is constant at constant pressure. Level control is often used for vaporizers: the controller controlling the steam supply to the heating surface,

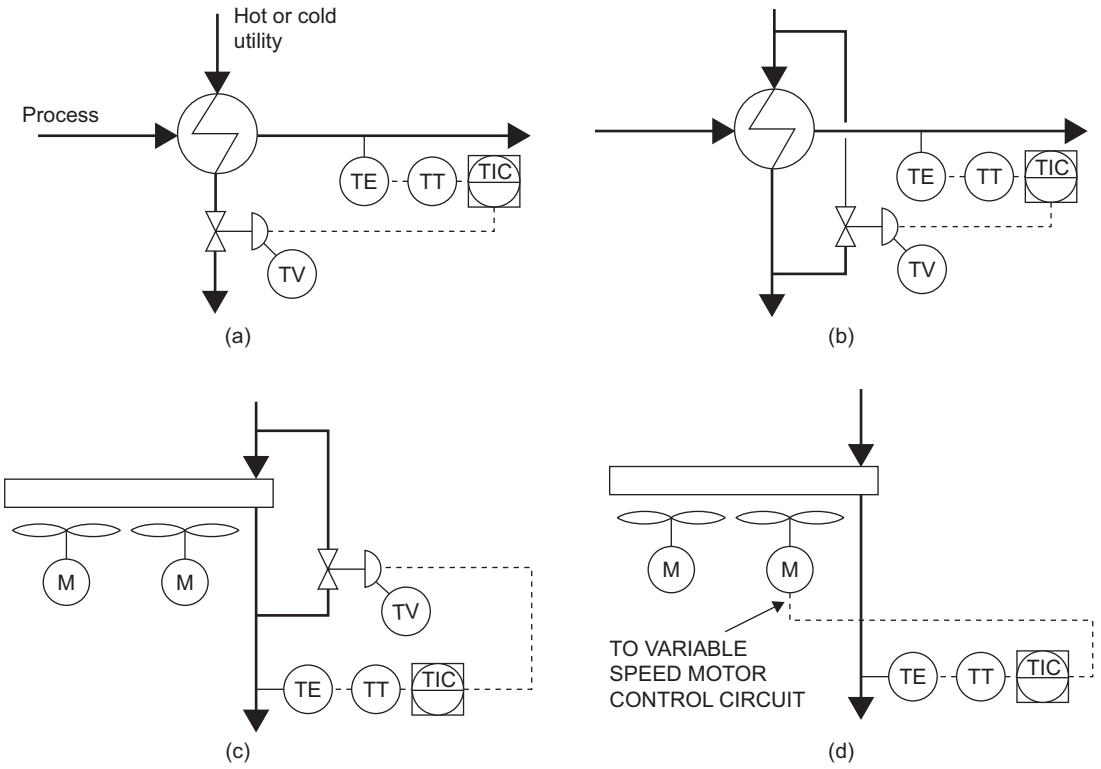


FIG. 5.12 (a) Temperature control of one fluid stream. (b) Bypass control. (c) Air cooler with bypass control. (d) Air cooler with variable-speed drive.

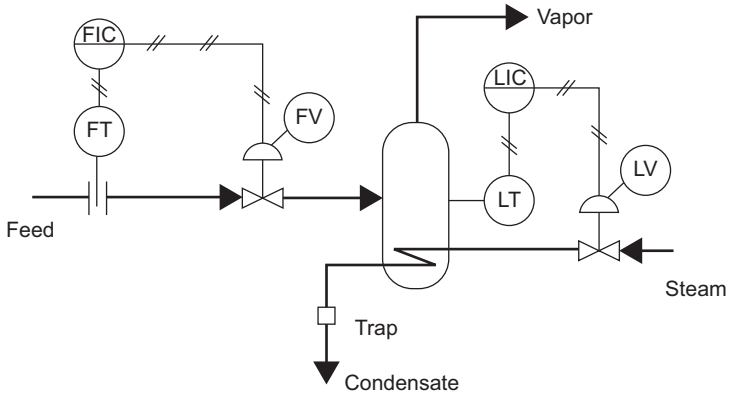


FIG. 5.13 Vaporizer control.

with the liquid feed to the vaporizer on flow control, as shown in Fig. 5.13. An increase in the feed results in an automatic increase in steam to the vaporizer to vaporize the increased flow and maintain a constant level.

Reboiler control systems are selected as part of the general control system for the distillation column and are discussed in Section 5.4.7.

5.4.5 Cascade control

With this arrangement, the output of one controller is used to adjust the set point of another. Cascade control can give smoother control in situations where direct control of the variable would lead to unstable operation. The secondary controller can be used to compensate for any short-term variations in, say, a utility stream flow, which would upset the controlled variable: the primary controller controlling long-term variations. Typical examples are shown in Figs. 5.18 and 5.19.

5.4.6 Ratio control

Ratio control can be used where it is desired to maintain two flows at a constant ratio, for example, reactor feeds or distillation column reflux. A typical scheme for ratio control is shown in Fig. 5.14.

5.4.7 Distillation column control

The primary objective of distillation column control is to maintain the specified composition of the top and bottom products and any side streams, correcting for the effects of disturbances in:

1. Feed flow rate, composition, and temperature
2. Steam or other hot utility supply
3. Cooling water or air cooler conditions
4. Ambient conditions, which can cause cooling of the column shell and changes in internal reflux (see Chapter 17)

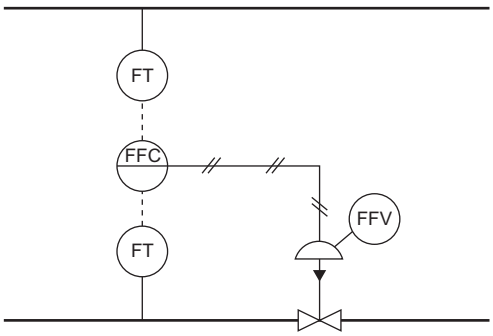


FIG. 5.14 Ratio control.

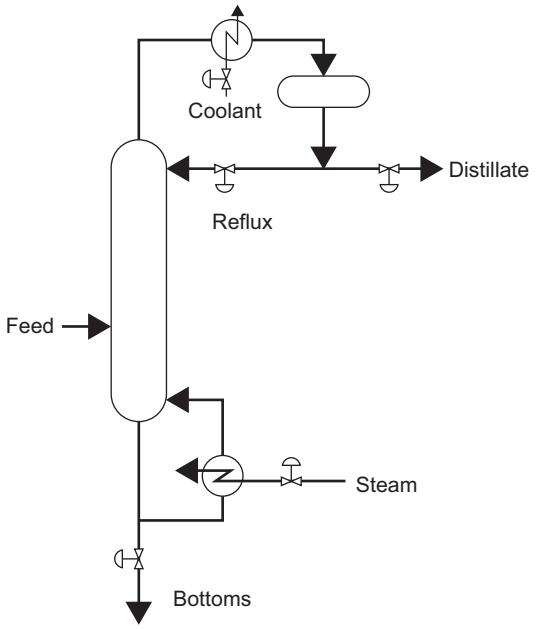


FIG. 5.15 Control valves and degrees of freedom for a simple distillation column.

The feed flow rate is often set by the level controller on a preceding column. It can be independently controlled if the column is fed from a storage or surge tank. Feed temperature is not normally controlled unless a feed pre-heater is used.

In the usual case where the feed rate is set by upstream operations and the column produces a liquid distillate product, there are five control valves, and hence five degrees of freedom; see Fig. 5.15. One degree of freedom is used to set the column pressure, usually by control of the condenser using one of the schemes shown in Fig. 5.10. Column pressure is normally controlled at a constant value, which then sets the vapor inventory in the column. The use of variable pressure control to conserve energy has been discussed by Shinskey (1976). Two degrees of freedom are needed to control the liquid inventories by controlling the vapor–liquid level in the column sump and the reflux drum (or condenser if no reflux drum is used).

The remaining two degrees of freedom can be used to achieve the desired separation, either in terms of product purity or recovery, by adjusting two flow rates. One of these flows is controlled by a flow or flow ratio controller to achieve the desired split between distillate and bottoms, while the other is usually controlled by a column temperature to achieve a desired composition in one of the products. The flow controller cannot be on the distillate or bottoms stream if the designer intends to control composition, as it would then be impossible to maintain product composition if there were changes in feed composition. The temperature controller can, however, control either the distillate or bottoms flow rate. The usual practice is to control a top temperature by varying the reflux ratio or distillate flow rate if the overhead product purity is more important (Fig. 5.16) to or control a bottom temperature by varying the boil-up rate or bottoms flow if bottoms purity is more important (Fig. 5.17).

Control schemes of this type are commonly referred to as *material balance* control schemes, as they achieve the desired product purity by manipulating the column material balance. These schemes are highly robust for processes where the feed flow rate to the column is relatively constant but the composition varies and close control must be maintained on one product composition.

Temperature is usually used as an indication of composition. The temperature sensor should be located at a position in the column where the rate of change of temperature with change in composition of the key component is a maximum; see Parkins (1959). Near the top and bottom of the column the change is usually small. When designing the column, it is a good idea to allow for thermowells on several trays so that the best control point can be found when the column is actually operating. If reliable online composition analyzers are available, they can be incorporated in the control loop, but more complex control equipment will be needed, and composition analyzers are usually used to cascade onto simpler temperature control loops. With multicomponent systems, temperature is not a unique function of composition.

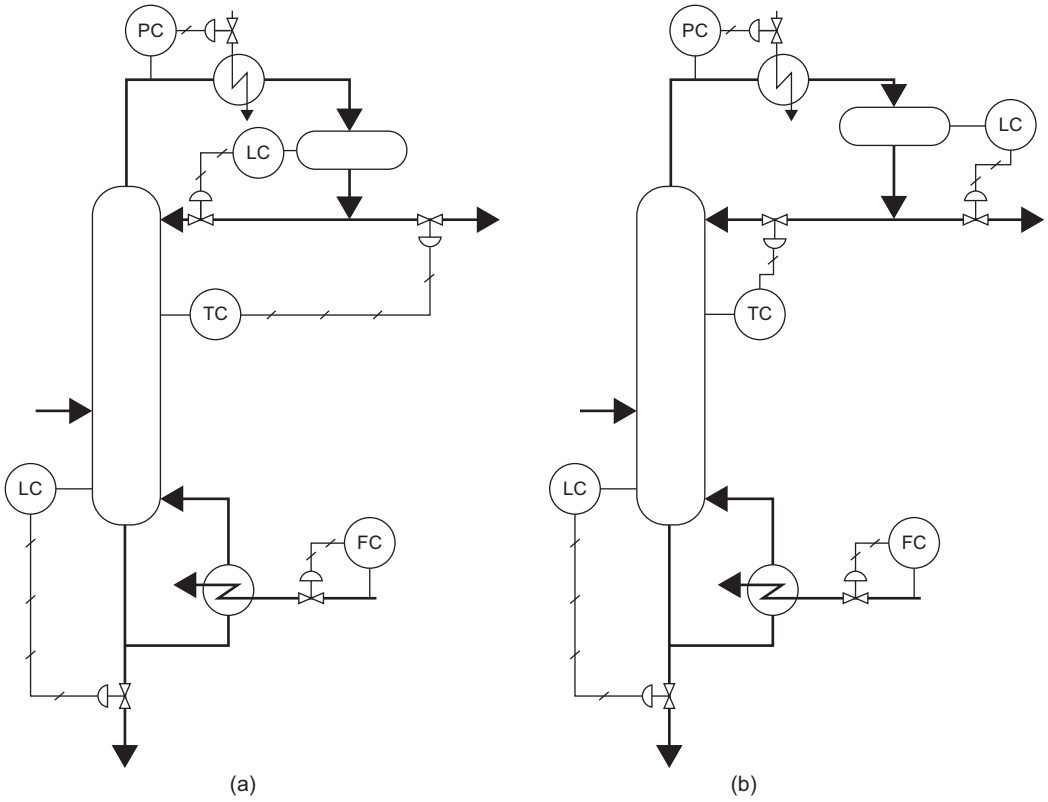


FIG. 5.16 Material balance control schemes for controlling overhead product composition. Flow control on reboiler can be in ratio to feed if feed rate varies. (a) Direct control of distillate by composition. (b) Indirect control of distillate; composition controls reflux.

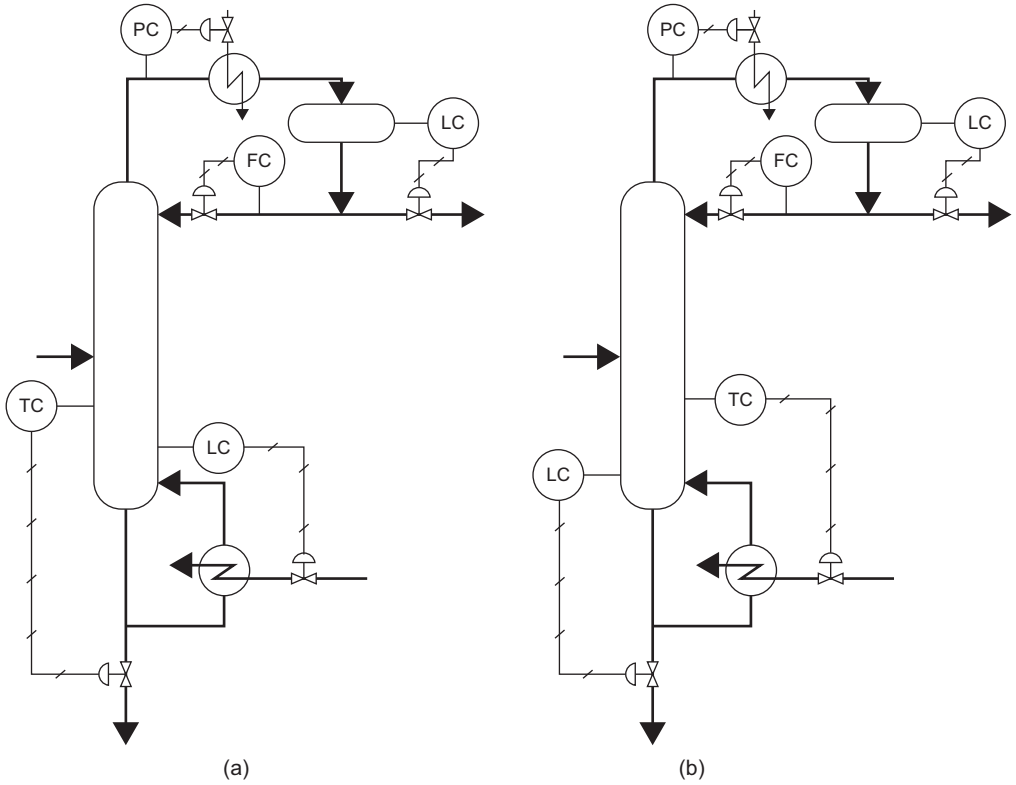


FIG. 5.17 Material balance control schemes for controlling bottoms product composition. Flow control on reflux can be in ratio to feed if feed rate varies. (a) Direct control of bottoms by composition. (b) Indirect control of bottoms; composition controls boil-up.

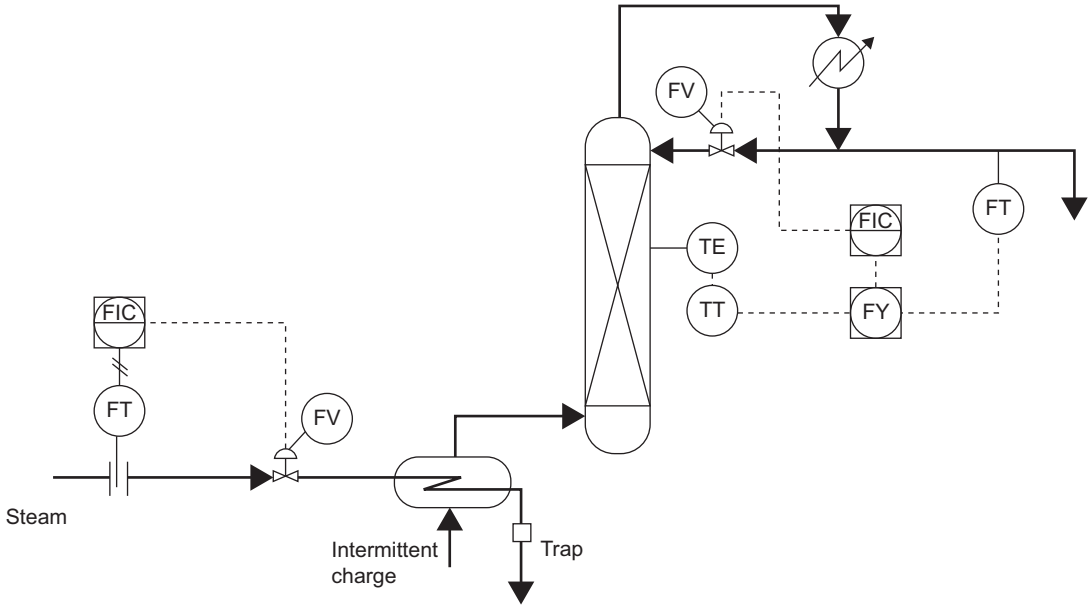


FIG. 5.18 Batch distillation, with reflux flow controlled based on temperature to infer composition.

Flow ratio controllers are sometimes used in distillation control, controlling the reflux or boil-up in ratio to the feed, distillate, or bottoms rate. The same effect can be accomplished using cascade control, with the feed rate adjusting the set point of the flow controller on reflux or boil-up.

Shinskey (1984) has shown that there are 120 ways of connecting the five main pairs of measured and controlled variables in single loops. A variety of control schemes has been devised for distillation column control. Some typical schemes are shown in Figs. 5.16 to 5.18; ancillary control loops and instruments are not shown.

The choice of control scheme may be influenced by many other factors. For example, the control scheme of Fig. 5.17b) controls boil-up by composition and gives the fastest control response to variations in composition of any of the schemes. Kister (1990) discusses the advantages and drawbacks of the material balance control schemes shown in Figs. 5.16 and 5.17.

An older control scheme that is often encountered is similar to Fig. 5.16(b) but has the steam to the reboiler controlled by a temperature in the stripping section of the column. This scheme is known as *temperature-pattern control* or *dual composition control*, and in principle allows both top and bottom compositions to be controlled. The drawback of this scheme is that there is a tendency for the controllers to fight each other, leading to unstable operation.

Distillation column control is discussed in detail by Parkins (1959), Bertrand and Jones (1961), Shinskey (1984), and Buckley et al. (1985).

Additional temperature indicating or recording points should be included up the column for monitoring column performance and for troubleshooting.

5.4.8 Reactor control

The schemes used for reactor control depend on the process and the type of reactor. If a reliable online composition analyzer is available and the reactor dynamics are suitable, the product composition can be monitored continuously and the reactor conditions and feed flows controlled automatically to maintain the desired product composition and yield. More often, the operator is the final link in the control loop, adjusting the controller set points to maintain the product within specification, based on periodic laboratory analyses.

For small stirred-tank reactors, temperature will normally be controlled by regulating the flow of the heating or cooling medium. For larger reactors, temperature is often controlled by recycling a part of the product stream or adding inert material to the feed to act as a heat sink. Pressure is usually held constant. For liquid phase reactors, pressure is often controlled by maintaining a vapor space above the liquid reagents. This space can be pressurized with nitrogen or other suitable gases. Material balance control will be necessary to maintain the correct flow of reactants to the reactor and the flow of products and unreacted materials from the reactor. A typical control scheme for a simple liquid phase reactor is shown in Fig. 5.19. See also Luyben (2007).

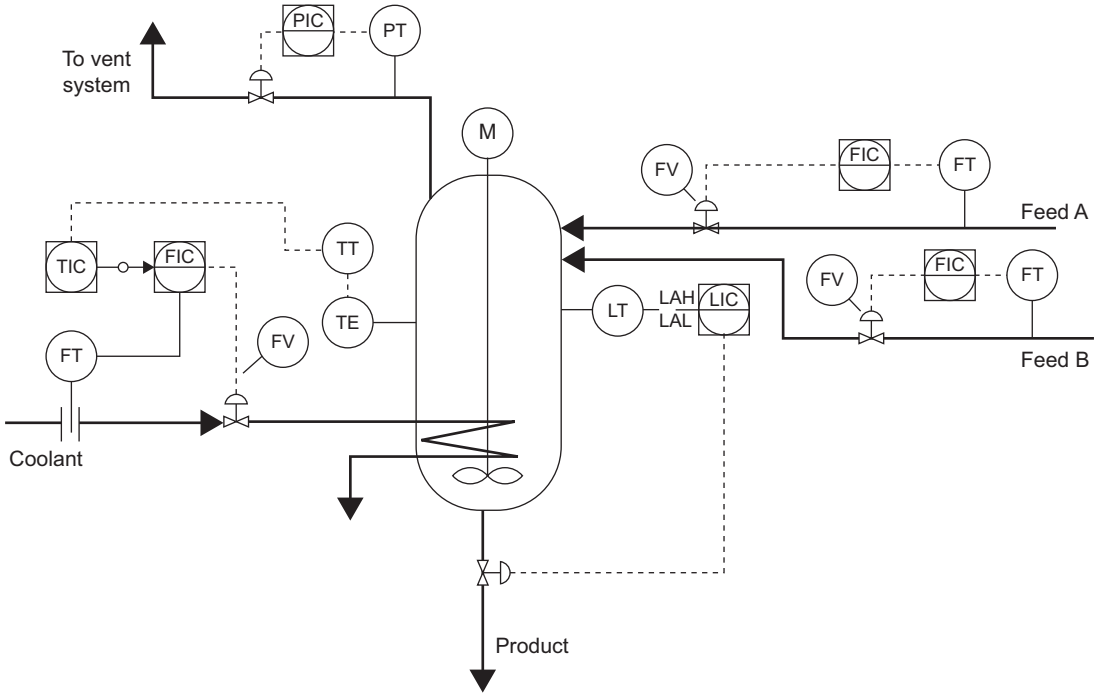


FIG. 5.19 A typical stirred tank reactor control scheme, temperature cascade control of coolant flow, and flow control of reagents.

The control of biological reactions is more complex because it is necessary to maintain many parameters within relatively tight ranges. Control of biological reactors is discussed in Section 15.9.7.

5.5 Alarms, safety trips, and interlocks

Alarms are used to alert operators to serious, and potentially hazardous, deviations in process conditions. Key instruments are fitted with switches and relays or software alarms to operate audible and visual alarms on the control panels and shared display screens. Where delay or lack of response by the operator is likely to lead to the rapid development of a hazardous situation, the instrument would be fitted with a trip system to take action automatically to avert the hazard, such as shutting down pumps, closing valves, and operating emergency systems.

The basic components of an automatic trip system are:

1. A sensor to monitor the control variable and provide an output signal when a preset value is exceeded (the instrument)
2. A link to transfer the signal to the actuator, usually consisting of a system of pneumatic or electric relays
3. An actuator to carry out the required action: close or open a valve, switch off a motor, etc.

A description of some of the equipment (hardware) used is given by Rasmussen (1975).

A safety trip can be incorporated in a control loop, as shown in Fig. 5.20(a). In this system the level control instrument has a built-in software alarm that alerts the operator if the level is too low and a programmed trip set for a level somewhat lower than the alarm level. However, the safe operation of such a system will be dependent on the reliability of the control equipment, and for potentially hazardous situations, it is better practice to specify a separate trip system, such as that shown in Fig. 5.20(b), in which the trip is activated by a separate low-level switch. Provision must be made for the periodic checking of the trip system to ensure that the system operates when needed.

The effective operation of instrumented safety systems depends on the reliable operation of all the components in the system. Because no component is perfectly reliable, designers increase the system reliability by building in redundancy and adding duplicate instruments, switches, relays, etc., so that if one component fails the rest of the system will still operate correctly. More information on the design of safety instrumented systems is given in Section 10.8.

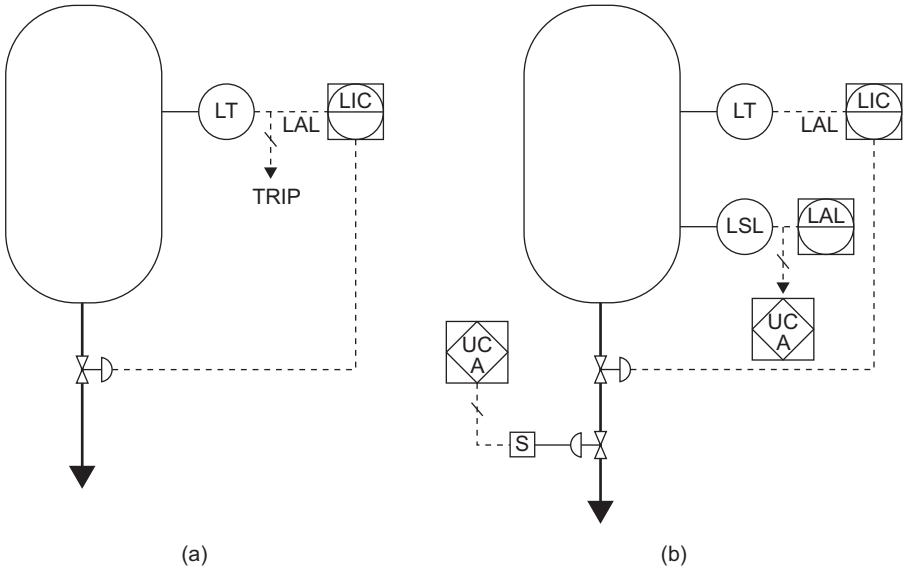


FIG. 5.20 (a) Trip as part of control system. (b) Separate shut-down trip.

Interlocks

Where it is necessary to follow a fixed sequence of operations—for example, during a plant start-up and shut-down, or in batch operations—interlocks are included to prevent operators from departing from the required sequence. They may be incorporated in the control system design, as pneumatic or electric relays, or may be mechanical interlocks. Various proprietary special lock and key systems are also available. In most plants, programmable logic controllers are used, and the interlocks are coded into the control algorithms. Care should be taken to test all of the interlocks in the plant automation during commissioning or whenever changes are made to the plant control and automation.

5.6 Batch process control

Batch processes necessarily involve dynamic variation in process parameters, and so the design of control systems for batch plants is more complex than for plants that operate continuously. In addition to conventional regulatory control functions that maintain temperatures, pressures, flows, and levels at desired values, the designer must consider discrete (on-off) control functions that start and stop operations, as well as the overall recipe or sequence of operations. In a plant that has several batch processes or that makes multiple products, the automation system may also include production planning, batch sequencing, and tracking and logging of batch data for quality control purposes.

The international standard for the design of control systems for batch plants is IEC 61512, which is based on the set of standards developed by the ISA S88 committee. These standards define an architecture for batch process control systems that regulates the flow of information from high-level decisions such as recipe management and production scheduling down to low-level regulatory process control functions. A detailed description of the S88 standards is beyond the scope of this book—for more information the reader should consult ISA 88.00.01 (2010) or the books by Fleming and Pillai (1998), Parshall and Lamb (2000), or Love (2007).

When developing a PFD or P&I diagram for a batch plant, the design team must consider all of the controllers that are needed to regulate the dynamic operation of the plant. The regulatory controllers will control the same variables that would be controlled in a continuous process. Indeed, during some phases of the batch recipe, the regulatory control loops function in the same way as they would for a continuous process. In addition to the regulatory control systems, the designer must then add the discrete control functions that change the set points of the regulatory controllers and activate the opening and closing of isolation valves to start and stop flows to the process. Microprocessor-based programmable logic controllers are usually used to control the sequence of phases that makes up the batch recipe.

5.7 Computer control systems

Almost all process control systems installed on new plants use programmable electronic devices based on microprocessors. These range from simple digitally actuated single-loop controllers that produce a single output signal (single input–single output [SISO] devices) up to complex distributed control systems that carry out control, real-time optimization, and data logging and archiving for multiple process plants across a site or even an enterprise (multiple input–multiple output [MIMO] devices).

The use of microprocessors in controllers allows the controllers to perform more complex control algorithms than could previously be achieved using analog systems based on pneumatic signals. A microprocessor can take input from several instruments and use a sophisticated model to calculate the outputs to multiple actuators. A simple example of a multiple input device is a gas mass-flow controller (Fig. 5.21), in which the gas mass flow is computed based on inputs from temperature, pressure, and flow instruments.

The conventional control schemes described in Section 5.4 mainly make use of SISO controllers, because the schemes were developed for single unit operations. At the unit operation level, the primary focus of process control is usually on safe and stable operation, and it is difficult to take full advantage of the capability of advanced microprocessor-based control systems. When several unit operations are put together to form a process, then the scope for use of MIMO devices increases, particularly when the devices are able to communicate with each other rapidly. The digital control system can then make use of more complex algorithms and models that enable feed-forward control (model-based or multivariable predictive control) and allow data collected from upstream in the process to guide the selection of operating conditions and controller set points for downstream operations. This allows for better response to process dynamics and more rapid operation of batch, cyclic, and other unsteady-state processes. Model-based predictive control is also often used as a means of controlling product quality. This is because devices for measuring product quality typically require analytical procedures that take several minutes to hours to run, making effective real-time feedback control difficult to accomplish.

The use of instruments that log and archive data facilitates remote monitoring of process performance and can improve plant troubleshooting and optimization, as well as providing high-level data for enterprise-wide supply chain management. Increasingly, archived data from plant historian databases is used to develop algorithms that predict safety and maintenance issues and allow more stable and economically efficient operation of the plant. These algorithms can be based on data from multiple sensing instruments and can be either deterministic (developed by regression of equations input by an engineer based on knowledge of engineering fundamentals) or fully empirical (developed by machine learning approaches).

The electronic equipment and systems technology available for process control continues to evolve rapidly. Because of the pace of innovation, industry-wide standards have not been able to keep up, and consequently different manufacturers' systems often use proprietary technology and are often not fully compatible with each other. The implementation of the ISA 50, ISA 100, HART Foundation Fieldbus, and OPC UA standards substantially improved digital communications between control devices, leading to improved control, faster set-up, better reliability through higher redundancy, and even greater distribution of functions between devices.

Wireless systems are beginning to be used in inventory control and maintenance management, but are not widely used yet in plant control. The control systems vendors have overcome problems with interference, signal blocking, and signal loss and have demonstrated robust error checking and transmission protocols. As experience is gained with wireless instrumentation, it is likely to be much more widely adopted in the future, as wireless systems are more convenient to install and can be more robust in the event of incidents such as small fires. A recent survey of wireless control was given by McKeon-Slattery (2010), but this area is currently evolving rapidly.

A detailed treatment of digital technology for process control is beyond the scope of this book. Kalani (1988), Edgar et al. (1997), Liptak (2012), and Love (2007) all provide excellent reviews of the subject. Mitchell and Law

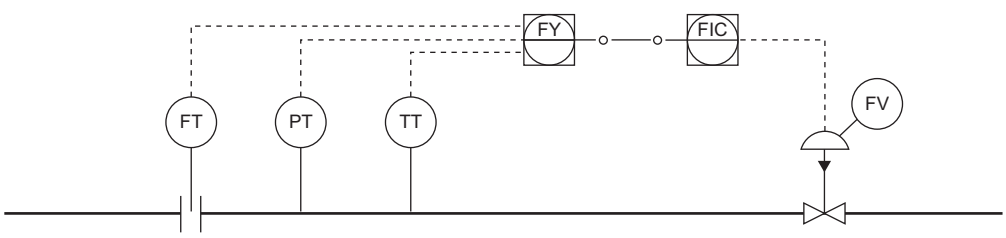


FIG. 5.21 Gas mass flow controller.

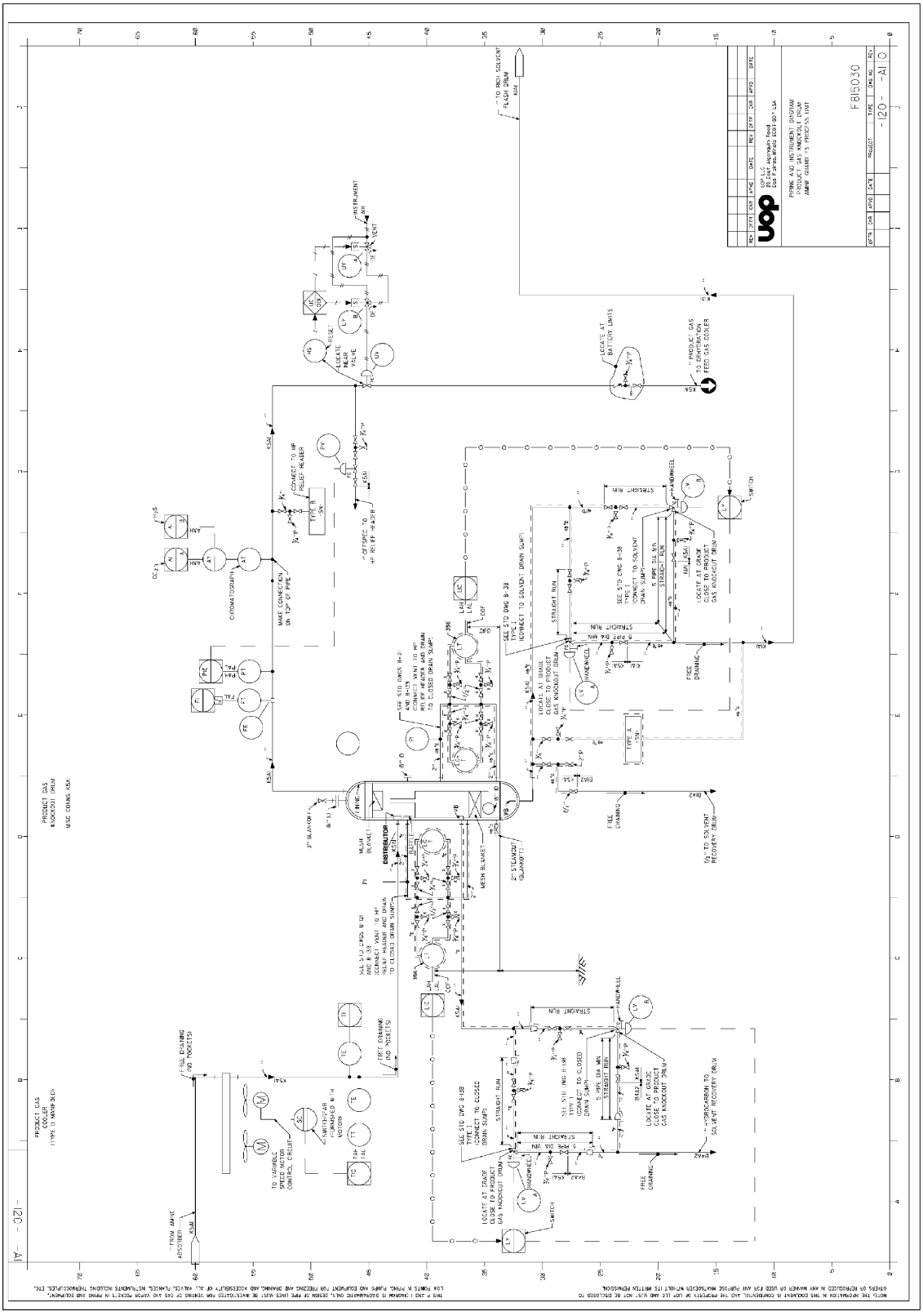


FIG. 5.22 Piping and instrumentation diagram.

(2003) give a good overview of digital bus technologies. Baldi (2016) discusses the cybersecurity defense of industrial control systems. Bagajewicz (2010) gives a comprehensive overview of issues in extracting real-time process data and using them to develop models for advanced control and process performance monitoring and optimization.

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5.9 Problems

5.1. How would you measure:

1. The temperature of a fermentation broth.
2. The mass flow of a gas at high temperature and pressure.
3. The volumetric flow rate of a slurry of diced carrots in water.
4. The level of liquid in a crystallizer.
5. The feed rate of solids to a mixing tank.

5.2. a. What alarms would you add to the vaporizer control scheme shown in Fig. 5.13? Indicate whether the alarm would signal high or low conditions, what the alarm would signify, and what operator response would be required in each case.
b. Which alarms should activate a shut-down trip, and which valves should be closed?

5.3. Sketch a control scheme for the reactor section shown in Fig. 2.17. The feeds are liquids, and the reactors operate under pressure with inert nitrogen in the vapor space above the reagents. The objective is to achieve full conversion of feed A by the outlet of the last reactor.

5.4. A fermentation reactor is charged with a sterile feed of growth media at 35 °C and inoculated with a batch of microorganism. The batch is allowed to grow for 10 days. During the growth period the temperature is maintained at 37 °C by circulating cold water through a jacket on the vessel. Sterile air is sparged into the fermenter to maintain a desired dissolved oxygen concentration. The pH of the fermenter is controlled by periodic addition of a dilute solution of sodium hydroxide. At the end of the growth period the batch is discharged from the reactor to the harvesting section of the process.
a. Sketch a P&I diagram of the reactor and feed section.
b. What pressure would you choose for operation of the fermenter, and how would you control it?

5.5. A polymer is produced by the emulsion polymerization of acrylonitrile and methyl methacrylate in a stirred vessel. The monomers and an aqueous solution of catalyst are fed to the polymerization reactor continuously. The product is withdrawn from the base of the vessel as a slurry.
Devise a control system for this reactor, and draw up a preliminary piping and instrument diagram. The following points need to be considered:

1. Close control of the reactor temperature is required.
2. The reactor runs 90% full.
3. The water and monomers are fed to the reactor separately.
4. The emulsion is a 30% mixture of monomers in water.
5. The flow of catalyst will be small compared with the water and monomer flows.
6. Accurate control of the catalyst flow is essential.

5.6. Devise a control system for the distillation column described in Chapter 17, Example 17.2. The flow to the column comes from a storage tank. The product, acetone, is sent to storage and the waste to an effluent pond. It is essential that the specifications on product and waste quality are met.

CHAPTER

6

Materials of construction

KEY LEARNING OBJECTIVES

- Mechanical and chemical properties that must be considered when selecting materials of construction for a chemical plant
- Relative costs of common materials of construction
- Properties of alloys commonly used in engineering
- When to use polymers or ceramic materials

6.1 Introduction

This chapter covers the selection of materials of construction for process equipment and piping. The selection of materials of construction must be made before the capital cost of a process can be estimated, as plant costs can vary significantly with materials selection.

Many factors have to be considered when selecting engineering materials, but for a chemical process plant, the overriding considerations are usually high temperature strength and the ability to resist corrosion. The process designer will be responsible for recommending materials that will be suitable for the process conditions. The process engineer must also consider the requirements of the mechanical design engineer; the material selected must have sufficient strength and be easily worked. The most economical material that satisfies both process and mechanical requirements should be selected; this will be the material that gives the lowest cost over the working life of the plant, allowing for maintenance and replacement. Other factors, such as product contamination and process safety, must also be considered. The mechanical properties that are important in the selection of materials are discussed briefly in this chapter. Several books have been published on the properties of materials and the metal-working processes used in equipment fabrication, and a selection suitable for further study is given in the list of references at the end of this chapter. The mechanical design of process equipment is discussed in Chapter 14.

A detailed discussion of the theoretical aspects of corrosion is not given in this chapter, as this subject is covered comprehensively in several books: Revie (2011), Fontana (1986), Dillon (1994), and Schweitzer (1989). An extensive set of corrosion data for different materials is given by Craig and Anderson (1995).

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6.2 Material properties

The most important characteristics to be considered when selecting a material of construction are:

1. Mechanical properties
   a. Strength: tensile strength
   b. Stiffness: elastic modulus (Young's modulus)
   c. Toughness: fracture resistance
   d. Hardness: wear resistance
   e. Fatigue resistance
   f. Creep resistance
2. The effect of high temperature, low temperature, and thermal cycling on the mechanical properties
3. Corrosion resistance
4. Any special properties required, such as thermal conductivity, electrical resistance, and magnetic properties
5. Ease of fabrication: forming, welding, casting (Table 6.1)
6. Availability in standard sizes: plates, sections, and tubes
7. Cost

TABLE 6.1 A guide to the fabrication properties of common metals and alloys

	Machining	Cold working	Hot working	Casting	Welding	Annealing temp.°C
Mild steel	S	S	S	D	S	750
Low alloy steel	S	D	S	D	S	750
Cast iron	S	U	U	S	D/U	—
Stainless steel (18 Cr, 8 Ni)	S	S	S	D	S	1050
Nickel	S	S	S	S	S	1150
Monel	S	S	S	S	S	1100
Copper (deoxidized)	D	S	S	S	D	800
Brass	S	D	S	S	S	700
Aluminum	S	S	S	D	S	550
Dural	S	S	S	—	S	350
Lead	—	S	—	—	S	—
Titanium	S	S	U	U	D	—

S, Satisfactory; D, Difficult, special techniques needed; U, Unsatisfactory.

6.3 Mechanical properties

Typical values of the mechanical properties of the more common materials used in the construction of chemical process equipment are given in Table 6.2.

6.3.1 Tensile strength

The tensile strength (tensile stress) is a measure of the basic strength of a material. It is the maximum stress that the material will withstand, measured by a standard tensile test. The older name for this property, which is more descriptive of the property, was ultimate tensile strength (UTS).

Proof stress is the stress that causes a specified permanent extension, usually 0.1%.

The maximum allowable stress specified by the ASME Boiler and Pressure Vessel (BPV) Code is calculated from these and other material properties at the design temperature, allowing for suitable safety factors. The basis for establishing maximum allowable stress values is discussed in Chapter 14 and is described in detail in the ASME BPV Code Section II Part D, Mandatory Appendix 1.

TABLE 6.2 Mechanical properties of common metals and alloys (typical values at room temperature)

	Tensile strength (N/mm^2)	0.1% proof stress (N/mm^2)	Modulus of elasticity (kN/mm^2)	Brinell hardness	Specific gravity
Mild steel	430	220	210	100–200	7.9
Low-alloy steel	420–660	230–460	210	130–200	7.9
Cast iron	140–170	—	140	150–250	7.2
Stainless steel (18 Cr, 8 Ni)	>540	200	210	160	8.0
Nickel (>99% Ni)	500	130	210	80–150	8.9
Monel	650	170	170	120–250	8.8
Copper (deoxidized)	200	60	110	30–100	8.9
Brass (admiralty)	400–600	130	115	100–200	8.6
Aluminum (>99%)	80–150	—	70	30	2.7
Dural	400	150	70	100	2.7
Lead	30	—	15	5	11.3
Titanium	500	350	110	150	4.5

Note: Tensile stress and proof stress are not the same as the maximum allowable stress permitted by design code. See Tables 6.5 and 6.7 for maximum allowable stress values.

6.3.2 Stiffness

Stiffness is the ability to resist bending and buckling. It is a function of the elastic modulus of the material and the shape of the cross-section of the member (the second moment of area).

6.3.3 Toughness

Toughness is associated with tensile strength, and is a measure of the material's resistance to crack propagation. The crystal structure of ductile materials, such as steel, aluminum, and copper, is such that they stop the propagation of a crack by local yielding at the crack tip. In other materials, such as the cast irons and glass, the structure is such that local yielding does not occur and the materials are brittle. Brittle materials are weak in tension but strong in compression. Under compression any incipient cracks present are closed up. Various techniques have been developed to allow the use of brittle materials in situations where tensile stress would normally occur—for example, the use of prestressed concrete and glass fiber–reinforced plastics in pressure vessel construction.

A detailed discussion of the factors that determine the fracture toughness of materials can be found in the books by the Institute of Metallurgists (1960) and Boyd (1970). Gordon (2018) gives an elementary, but very readable, account of the strength of materials in terms of their macroscopic and microscopic structure.

6.3.4 Hardness

The surface hardness, as measured in a standard test, is an indication of a material's ability to resist wear. This will be an important property if the equipment is being designed to handle abrasive solids or liquids containing suspended solids that are likely to cause erosion.

6.3.5 Fatigue

Fatigue failure is likely to occur in equipment subject to cyclic loading, for example, rotating equipment, such as pumps and compressors, and equipment subjected to temperature or pressure cycling. A comprehensive treatment of this subject is given by Harris (1976).

6.3.6 Creep

Creep is the gradual extension of a material under a steady tensile stress over a prolonged period. It is usually only important at high temperatures, for instance, with steam and gas turbine blades. For a few materials, notably lead, the rate of creep is significant at moderate temperatures. Lead will creep under its own weight at room temperature, and lead linings must be supported at short intervals.

The creep strength of a material is usually reported as the stress to cause rupture in 100,000 hours at the test temperature.

6.3.7 Effect of temperature on the mechanical properties

The tensile strength and elastic modulus of metals decrease with increasing temperature. For example, the tensile strength of mild steel (low-carbon steel, C <0.25 %) is 450 N/mm^2 at 25 °C, falling to 210 N/mm^2 at 500 °C, and the value of Young's modulus is 200,000 N/mm^2 at 25 °C, falling to 150,000 N/mm^2 at 500 °C. The ASME BPV Code Section II Part D specifies maximum temperatures for each material. For example, SA-285 plain carbon steel plate cannot be used to construct a pressure vessel that meets the specifications of ASME BPV Code Section VIII Div. 1 with a design temperature greater than 482 °C (900 °F). Any pressure vessel that is designed for use above this temperature must be made from killed steel or alloy. The maximum allowable stress used in a design is always based on the design temperature. Materials must be chosen that have sufficient strength at the design temperature to give an economic and mechanically feasible wall thickness. The stainless steels are superior in this respect to plain carbon steels.

Creep resistance will be important if the material is subjected to high stresses at elevated temperatures. Special alloys, such as Inconel 600 (UNS N06600) or Incoloy 800 (UNS N08800) (both trademarks of International Nickel Co.) are used for high-temperature equipment such as furnace tubes in environments that do not contain sulfur. The selection of materials for high-temperature applications is discussed by Day (1979) and Lai (1990).

At low temperatures, less than 10 °C, metals that are normally ductile can fail in a brittle manner. Serious disasters have occurred through the failure of welded carbon steel vessels at low temperatures. The phenomenon of brittle failure is associated with the crystalline structure of metals. Metals with a body-centered-cubic (bcc) lattice are more liable to brittle failure than those with a face-centered-cubic (fcc) or hexagonal lattice. For low-temperature equipment, such as cryogenic plant and liquefied-gas storages, austenitic stainless steel (fcc) or aluminum alloys (hex) should be specified; see Wigley (1978).

V-notch impact tests, such as the Charpy test, are used to test the susceptibility of materials to brittle failure: see Wells (1968) and ASME BPV Code Sec. VIII Div. 1 Part UG-84.

The brittle fracture of welded structures is a complex phenomenon and is dependent on plate thickness and the residual stresses present after fabrication, as well as the operating temperature. A comprehensive discussion of brittle fracture in steel structures is given by Boyd (1970).

6.4 Corrosion resistance

The conditions that cause corrosion can arise in a variety of ways. For this brief discussion on the selection of materials, it is convenient to classify corrosion into the following categories:

1. General wastage of material – uniform corrosion
2. Galvanic corrosion – dissimilar metals in contact
3. Pitting – localized attack
4. Intergranular corrosion
5. Stress corrosion
6. Erosion – corrosion
7. Corrosion fatigue
8. High-temperature oxidation and sulfidation
9. Hydrogen embrittlement

Metallic corrosion is essentially an electrochemical process. Four components are necessary to set up an electrochemical cell:

1. Anode – the corroding electrode
2. Cathode – the passive, noncorroding electrode

3. The conducting medium (the electrolyte) – the corroding fluid
4. Completion of the electrical circuit through the material

Cathodic areas can arise in many ways:

1. Dissimilar metals
2. Corrosion products
3. Inclusions in the metal, such as slag
4. Less well-aerated areas
5. Areas of differential concentration
6. Differentially strained areas

6.4.1 Uniform corrosion

This term describes the more or less uniform wastage of material by corrosion, with no pitting or other forms of local attack. If the corrosion of a material can be considered to be uniform, the life of the material in service can be predicted from experimentally determined corrosion rates.

Corrosion rates are usually expressed as a penetration rate in inches per year, or mills per year (mpy) (where a mill $= 10^{-3}$ inches). They are also expressed as a weight loss in milligrams per square decimeter per day (mdd). Most of the published data on corrosion rates are in imperial units. In corrosion testing, the corrosion rate is measured by the reduction in weight of a specimen of known area over a fixed period.

$$\text{ipy} = \frac{12w}{tA\rho} \tag{6.1}$$

where w = mass loss in time t, lb
t = time, years
A = surface area, ft^2
ρ = density of material, lb/ft^3

In SI units 1 ipy = 25 mm per year.

When judging corrosion rates expressed in mdd, it must be remembered that the penetration rate depends on the density of the material. For ferrous metals 100 mdd = 0.02 ipy.

What can be considered an acceptable rate of attack will depend on the cost of the material; the duty, particularly with regard to safety; and the economic life of the plant. For the more commonly used inexpensive materials, such as the carbon and low-alloy steels, a guide to what is considered acceptable is given in Table 6.3. For the more expensive alloys, such as the high-alloy steels, the brasses, and aluminum, the figures given in Table 6.3 should be divided by 2.

If the predicted corrosion rate indicates only short exposures, the design engineer should allow for frequent inspection of the plant and periodic replacement of the affected equipment. This affects process economics in two ways, as it reduces the on-stream factor (number of days of production per year) and increases the maintenance costs. Usually the economic impact of frequent shut-down and replacement is so negative that use of a more expensive alloy with better corrosion resistance can be justified.

Allowances for expected corrosion over the plant life or time between replacements must be added to the minimum vessel wall thicknesses calculated to comply with the ASME BPV Code. These corrosion allowances

TABLE 6.3 Acceptable corrosion rates

	Corrosion rate	
	ipy	**mm/y**
Completely satisfactory	<0.01	0.25
Use with caution	<0.03	0.75
Use only for short exposures	<0.06	1.5
Completely unsatisfactory	>0.06	1.5

can be economically or mechanically prohibitive if the corrosion rate is high. Guidance on corrosion allowances is given in the ASME BPV Code Sec. VIII Div. 1 Non-mandatory Appendix E. The corrosion allowance should at least equal the expected corrosion loss during the desired life of the vessel.

The corrosion rate will be dependent on the temperature and concentration of the corrosive fluid. An increase in temperature usually results in an increased rate of corrosion, though not always. The rate will depend on other factors that are affected by temperature, such as oxygen solubility.

The effect of concentration can also be complex—for example, the corrosion of mild steel in sulfuric acid, where the rate is unacceptably high in dilute acid and at concentrations above 70%, but is acceptable at intermediate concentrations.

6.4.2 Galvanic corrosion

If dissimilar metals are placed in contact, in an electrolyte, the corrosion rate of the anodic metal will be increased, as the metal lower in the electrochemical series will readily act as a cathode. The galvanic series in sea water for some of the more commonly used metals is shown in Table 6.4. Some metals under certain conditions form a natural protective film, for example, stainless steel in oxidizing environments. This state is denoted by "passive" in the series shown in Table 6.4. Active indicates the absence of the protective film, for example, where the surface of the metal is subject to wear due to moving parts or abrasion by the fluid. Minor shifts in position in the series can be expected in other electrolytes, but the series for sea water is a good indication of the combinations of metals to be avoided. If metals that are widely separated in the galvanic series have to be used together, they should be electrically insulated from each other, breaking the conducting circuit. Alternatively, if sacrificial loss of the anodic material can be accepted, the thickness of this material can be increased to allow for the increased rate of corrosion. The corrosion rate will depend on the relative areas of the anodic and cathodic metals. A high cathode to anode area should be avoided. Sacrificial anodes are used to protect underground steel pipes.

TABLE 6.4 Galvanic series in sea water

Noble end (protected end)	18/8 stainless steel (passive)
	Monel
	Inconel (passive)
	Nickel (passive)
	Copper
	Aluminum bronze (Cu 92%, Al 8%)
	Admiralty brass (Cu 71%, Zn 28%, Sn 1%)
	Nickel (active)
	Inconel (active)
	Lead
	18/8 stainless steel (active)
	Cast iron
	Mild steel
	Aluminum
	Galvanized steel
	Zinc
	Magnesium

6.4.3 Pitting

Pitting is the term given to highly localized corrosion that forms pits in the metal surface. If a material is liable to pitting, penetration can occur prematurely, and corrosion rate data are not a reliable guide to the equipment life.

Pitting can be caused by a variety of circumstances; any situation that causes a localized increase in corrosion rate may result in the formation of a pit. In an aerated medium the oxygen concentration will be lower at the bottom of a pit, and the bottom will be anodic to the surrounding metal, causing increased corrosion and deepening of the pit. A good surface finish will reduce this type of attack. Pitting can also occur if the composition of the metal is not uniform, for example, the presence of slag inclusions in welds. The impingement of bubbles can also cause pitting, as seen when cavitation occurs in pumps, which is an example of erosion-corrosion.

6.4.4 Intergranular corrosion

Intergranular corrosion is the preferential corrosion of material at the grain (crystal) boundaries. Though the loss of material will be small, intergranular corrosion can cause the catastrophic failure of equipment. Intergranular corrosion is a common form of attack on alloys but occurs rarely with pure metals. The attack is usually caused by a differential couple being set up between impurities existing at the grain boundary. Impurities will tend to accumulate at the grain boundaries after heat treatment. The classic example of intergranular corrosion in a chemical plant is the weld decay of unestablished stainless steel. This is caused by the precipitation of chromium carbides at the grain boundaries in a zone adjacent to the weld, where the temperature has been between 500° and 800 °C during welding. Weld decay can be avoided by annealing after welding, if practical (postweld heat treatment) or by using low carbon grades (<0.3% C) or grades stabilized by the addition of titanium or niobium.

6.4.5 Effect of stress

Corrosion rate and the form of attack can be changed if the material is under stress. Generally, the rate of attack will not change significantly within normal design stress values; however, for some combinations of metal, corrosive media, and temperature, the phenomenon called *stress corrosion cracking* can occur. This is the general name given to a form of attack in which cracks are produced that grow rapidly and can cause premature, brittle failure of the metal. The conditions necessary for stress corrosion cracking to occur are:

1. Simultaneous stress and corrosion
2. A specific corrosive substance, in particular, the presence of Cl^-, OH^-, NO_3^-, or NH_4^+ ions

Mild stress can cause cracking; the residual stresses from fabrication and welding are sufficient. For a general discussion of the mechanism of stress corrosion cracking, see Fontana (1986). Some classic examples of stress corrosion cracking are:

- The season cracking of brass cartridge cases
- Caustic embrittlement of steel boilers
- The stress corrosion cracking of stainless steels in the presence of chloride ions

Stress corrosion cracking can be avoided by selecting materials that are not susceptible in the specific corrosion environment or, less certainly, by stress relieving by postweld heat treatment.

Comprehensive tables of materials susceptible to stress corrosion cracking in specific chemicals are given by Moore (1979). Moore's tables are taken from the corrosion data survey published by Hamner (1974). See also ASME BPV Code Sec. II Part D Appendix A-330.

The term *corrosion fatigue* is used to describe the premature failure of materials in corrosive environments caused by cyclic stresses. Even mildly corrosive conditions can markedly reduce the fatigue life of a component. Unlike stress corrosion cracking, corrosion fatigue can occur in any corrosive environment and does not depend on a specific combination of corrosive substance and metal. Materials with a high resistance to corrosion must be specified for critical components subjected to cyclic stresses.

6.4.6 Erosion-corrosion

The term *erosion-corrosion* is used to describe the increased rate of attack caused by a combination of erosion and corrosion. If a fluid stream contains suspended particles, or where there is high velocity or turbulence, erosion will

tend to remove the products of corrosion and any protective film, and the rate of attack will be markedly increased. If erosion is likely to occur, more resistant materials must be specified, or the material surface must be protected in some way. For example, plastic inserts can be used to prevent erosion-corrosion at the inlet to heat exchanger tubes.

6.4.7 High-temperature oxidation and sulfidation

Corrosion is normally associated with aqueous solutions, but oxidation can occur in dry conditions. Carbon steels and low-alloy steels will oxidize rapidly at high temperatures, and their use is limited to temperatures below 480 °C (900 °F).

Chromium is the most effective alloying element to give resistance to oxidation, forming a tenacious oxide film. Chromium alloys should be specified for equipment subject to temperatures above 480 °C in oxidizing atmospheres. For example, type 304L stainless steel (18% Cr) can be used up to 650 °C (1200 °F). For temperatures above 700 °C additional stabilization is needed. Type 347 stainless steel is stabilized with niobium and can be used up to 850 °C. High-nickel alloys can also be used as long as sulfur is not present, and high-chromium-content Ni alloys are used at the highest temperatures. For example, Inconel 600 (15.5% Cr) can be used up to 650 °C (1200 °F) and Incoloy 800 (21% Cr) can be used up to 850 °C (1500 °F).

Sulfur is a common corrosive contaminant in gas processing, oil refining, and energy conversion. In reducing environments sulfur is present as H_2S, which causes sulfidation of metals. The metal chosen must often withstand a sulfidizing environment on one side and an oxidizing environment on the other side, all at high temperature (for example, in a furnace tube). Sulfur can attack the chromium oxide scale that protects the alloy, causing breakaway corrosion, particularly for high-nickel alloys. Lai (1990) gives high-temperature corrosion data for various sulfidizing and mixed-gas environments and recommends the use of high-chromium, high-silicon alloys such as HR-160 in this service.

6.4.8 Hydrogen embrittlement

Hydrogen embrittlement is the name given to the loss of ductility caused by the absorption (and reaction) of hydrogen in a metal. It is of particular importance when specifying steels for use in a hydrogen reforming plant. Alloy steels have a greater resistance to hydrogen embrittlement than the plain carbon steels. A chart showing the suitability of various alloy steels for use in hydrogen atmospheres as a function of hydrogen partial pressure and temperature is given in the corrosion data survey by Hamner (1974). Below 500 °C plain carbon steel can be used.

6.5 Selection for corrosion resistance

To select the correct material of construction, the process environment to which the material will be exposed must be clearly defined. In addition to the main corrosive chemicals present, the following factors must be considered:

1. Temperature – affects corrosion rate and mechanical properties
2. Pressure
3. pH
4. Presence of trace impurities – stress corrosion
5. The amount of aeration – differential oxidation cells
6. Stream velocity and agitation – erosion-corrosion
7. Heat transfer rates – differential temperatures

The conditions that may arise during abnormal operation, such as at start-up and shut-down, must be considered in addition to normal, steady-state operation.

6.5.1 Corrosion charts

The resistance of some commonly used materials to a range of chemicals is shown in Appendix B, which is available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793. More comprehensive corrosion data, covering most of the materials used in the construction of a process plant, in a wide range of corrosive media, are given by Rabald (1968), NACE (2012), Hamner (1974), Green and Southard (2018), Lai (1990), and Schweitzer (1989, 2004, 2006). The 12-volume *Dechema Corrosion Handbook* is an extensive

guide to the interaction of corrosive media with materials (Kreysa and Schütze, 2007). The ASM *Handbook of Corrosion Data* also has extensive data (Craig and Anderson, 1995).

These corrosion guides can be used for the preliminary screening of materials that are likely to be suitable, but the fact that published data indicate that a material is satisfactory cannot be taken as a guarantee that it will be suitable for the process environment being considered. Slight changes in the process conditions, or the presence of unsuspected trace impurities, can markedly change the rate of attack or the nature of the corrosion. The guides will, however, clearly show those materials that are manifestly unsuitable. Judgment, based on experience with the materials in similar process environments, must be used when assessing published corrosion data.

Pilot plant tests and laboratory corrosion tests under simulated plant conditions will help in the selection of suitable materials if actual plant experience is not available. Preliminary tests can be carried out by inserting coupons of different materials into an apparatus that is known to resist corrosion and not cause galvanic effects before testing plant components. This reduces the likelihood of component failure and possible release of chemicals during testing. Care is needed in the interpretation of laboratory tests.

The advice of the technical service department of the company supplying the materials should also be sought.

6.6 Material costs

An indication of the cost of some commonly used metals is given in Table 6.5. The actual cost of metals and alloys will fluctuate quite widely, depending on movements in the world metal exchanges.

Current metals prices can be found at:

www.steelonthenet.com Free site with monthly carbon steel prices
www.steelbb.com Steel business briefing − subscription site with weekly carbon steel and stainless steel prices
www.steelweek.com Subscription site with weekly international prices
http://metalprices.com Great alloy calculator − 3-month-old prices are free; current prices are subscription only

The quantity of a material used will depend on the material density and strength (maximum allowable stress), and these must be taken into account when comparing material costs. Moore (1970) compares costs by calculating a cost rating factor defined by the equation:

$$\text{Cost rating} = \frac{C \times \rho}{\sigma_d} \tag{6.2}$$

where C = cost per unit mass, \$/kg
ρ = density, kg/m^3
σ_d = maximum allowable stress, N/mm^2

TABLE 6.5 Relative cost of metals (November 2010)

Metal	Type or grade	Price (\$/lb)	Max allowable stress (ksi = 1000 psi)	Relative cost rating
Carbon steel	A285	0.37	12.9	1
Austenitic stainless steel	304	1.156	20	2.0
	316	1.721	20	3.0
Copper	C10400	3.83	6.7	22.8
Aluminum alloy	AO3560	1.0789	8.6	1.5
Nickel	99% Ni	9.861	10	39.2
Incoloy	N08800	3.733	20	6.7
Monel	N04400	7.76	18.7	16.4
Titanium	R50250	3.35	10	6.8

Note: The maximum allowable stress values are at 40 °C (100 °F) and are taken from ASME BPV Code Sec. II Part D. The code should be consulted for values at other temperatures. Several other grades exist for most of the materials listed.

Cost ratings relative to the rating for mild steel (low carbon) are shown in Table 6.5 for November 2010 prices. Materials with a relatively high maximum allowable stress, such as stainless and low-alloy steels, can be used more efficiently than carbon steel. Note that the simplified formula given in Equation 6.2 does not take into account different corrosion allowances for the different materials.

The relative cost of equipment made from different materials will depend on the cost of fabrication, as well as the basic cost of the material. Unless a particular material requires special fabrication techniques, the relative cost of the finished equipment will be lower than the relative bare material cost. For example, the purchased cost of a stainless steel storage tank will typically be 2 to 3 times the cost of the same tank in carbon steel, whereas the relative cost of the metals is typically from 3 to 8.

If the corrosion rate is uniform, the optimum material can be selected by calculating the annual costs for the possible candidate materials. The annual cost will depend on the predicted life, calculated from the corrosion rate, and the purchased cost of the equipment. In a given situation, it may prove more economic to install a cheaper material with a high corrosion rate and replace it frequently rather than select a more resistant but more expensive material. This strategy would only be considered for relatively simple equipment with low fabrication costs and where premature failure would not cause a serious hazard. For example, carbon steel could be specified for an aqueous effluent line in place of stainless steel, accepting the probable need for replacement. The pipe wall thickness would be monitored *in situ* frequently, to determine when replacement was needed.

The more expensive, corrosion-resistant alloys are often used as a cladding on carbon steel. If a thick plate is needed for structural strength, as for pressure vessels, the use of clad materials can substantially reduce the cost. The design requirements for pressure vessels with cladding or applied internal linings are given in ASME BPV Code Sec. VIII Div. 1 Part UCL.

6.7 Contamination

With some processes, the prevention of the contamination of a process stream, or a product, by certain metals or the products of corrosion overrides any other considerations when selecting suitable materials. For instance, in textile processes, stainless steel or aluminum is often used in preference to carbon steel, which would be quite suitable except that any slight rusting will mark the textiles (iron staining).

With processes that use catalysts, care must be taken to select materials that will not cause contamination and poisoning of the catalyst.

Stainless steels are preferred in biological processes to reduce contamination by corrosion products. Copper alloys were used historically, but have been shown to inhibit fermentation. Most fermentation plants are built from 316 stainless steel, but 304 stainless steel is widely used in food processing applications.

Some other examples that illustrate the need to consider the effect of contamination by trace quantities of other materials are:

1. For equipment handling acetylene, the pure metals, or alloys containing copper, silver, mercury or gold, must be avoided to prevent the formation of explosive acetylides.
2. The presence of trace quantities of mercury in a process stream can cause the catastrophic failure of brass heat exchanger tubes as a result of the formation of a mercury−copper amalgam. Incidents have occurred where the contamination has come from unsuspected sources, such as the failure of mercury-in-steel thermometers.
3. In the Flixborough disaster, there was evidence that the stress corrosion cracking of a stainless steel pipe had been caused by zinc contamination from galvanized wire supporting lagging.

6.7.1 Surface finish

In industries such as the food, pharmaceutical, biochemical, and textile industries, the surface finish of the material is as important as the choice of material to avoid contamination.

Stainless steel is widely used, and the surfaces, inside and out, are given a high finish by abrasive blasting and mechanical polishing. This is done for the purposes of hygiene, to prevent material adhering to the surface, and to aid cleaning and sterilization. The surface finishes required in food processing are discussed by Timperley (1984) and Jowitt (1980).

A good surface finish is important in textile fiber processing to prevent the fibers from snagging.

6.8 Commonly used materials of construction

The general mechanical properties, corrosion resistance, and typical areas of use of some of the materials commonly used in the construction of chemical plant are given in this section. The values given are for a typical, representative grade of the material or alloy. The alloys used in chemical plant construction are known by a variety of trade names, and code numbers are designated in the various national standards. With the exception of the stainless steels, no attempt has been made in this book to classify the alloys discussed by using one or other of the national standards; the commonly used, generic names for the alloys have been used. For the full details of the properties and compositions of the different grades available in a particular class of alloy, and the designated code numbers, reference should be made to the appropriate national code, to the various handbooks, or to manufacturers' literature. See, for example, ASME BPV Code Sec. II Part D for a full listing of materials properties and ASME BPV Code Sec. VIII Div.1 for material-specific fabrication guidelines.

The U.S. trade names and codes are given by Green and Southard (2018). Comprehensive reviews of the engineering materials used for chemical and process plants can be found in the books by Evans (1980) and Hansen and Puyear (1996).

6.8.1 Iron and steel

Low-carbon steel (mild steel) is the most commonly used engineering material. It is cheap, is available in a wide range of standard forms and sizes, and can be easily worked and welded. It has good tensile strength and ductility.

The carbon steels and iron are not resistant to corrosion, except in certain specific environments, such as concentrated sulfuric acid and the caustic alkalis. They are suitable for use with most organic solvents, except chlorinated solvents, but traces of corrosion products may cause discoloration. Mild steel is susceptible to stress-corrosion cracking in certain environments.

The corrosion resistance of the low-alloy steels (less than 5% of alloying elements), where the alloying elements are added to improve the mechanical strength and not for corrosion resistance, is not significantly different from that of the plain carbon steels. Low-alloy steels are widely used in plants that process hydrocarbons at moderate temperatures, for example, in oil refining.

A comprehensive reference covering the properties and application of steels, including the stainless steels, is the book by Llewellyn and Hudd (1998). The use of carbon steel in the construction of chemical plants is discussed by Clark (1970).

The high-silicon irons (14% to 15% Si) have a high resistance to mineral acids, except hydrofluoric acid. They are particularly suitable for use with sulfuric acid at all concentrations and temperatures. They are, however, very brittle.

6.8.2 Stainless steel

The stainless steels are the most frequently used corrosion-resistant materials in the chemical industry.

To impart corrosion resistance, the chromium content must be above 12%, and the higher the chromium content, the more resistant the alloy is to corrosion in oxidizing conditions. Nickel is added to improve the corrosion resistance in nonoxidizing environments.

Types

A wide range of stainless steels is available, with compositions tailored to give the properties required for specific applications. They can be divided into three broad classes according to their microstructure:

1. Ferritic: 13% to 20% Cr, <0.1% C, with no nickel
2. Austenitic: 18% to 20% Cr, >7% Ni
3. Martensitic: 12% to 10% Cr, 0.2% to 0.4% C, up to 2% Ni

The uniform structure of austenite (fcc, with the carbides in solution) is the structure desired for corrosion resistance, and it is these grades that are widely used in the chemical industry. The compositions of the main grades of austenitic steels are shown in Table 6.6. Their properties are discussed next.

TABLE 6.6 Commonly used grades of austenitic stainless steel

Specification no.	Composition %							
AISI No.	**C max**	**Si Max**	**Mn Max**	**Cr Range**	**Ni Range**	**Mo Range**	**Ti**	**Nb**
304	0.08	—	2.00	17.5 20.0	8.0 11.0	—	—	—
304L	0.03	1.00	2.00	17.5 20.0	8.0 12.0	—	—	—
321	0.12	1.00	2.00	17.0 20.0	9.0 12.0	—	4 × C	—
347	0.08	1.00	2.00	17.0 20.0	9.0 13.0	—	—	10 × C
316	0.08	1.00	2.00	16.0 18.0	10.0 14.0	2.0 3.0	—	—
316L	0.03	1.0	2.0	16.0 18.0	10.0 14.0	2.0 3.0	—	—
309	0.20	—	—	22.0 24.0	12.0 15.0	—	—	—
310	0.25	—	—	24.0 26.0	19.0 22.0	—	—	—

S and P 0.045% all grades.
AISI, *American Iron and Steel Institute*.

- Type 304 (the so-called *18/8 stainless steels*): The most generally used stainless steel. It contains the minimum Cr and Ni that give a stable austenitic structure. The carbon content is low enough for heat treatment not to be normally needed with thin sections to prevent weld decay (see Section 6.4.4).
- Type 304L: Low-carbon version of type 304 (<0.03% C) used for thicker welded sections, where carbide precipitation would occur with type 304.
- Type 321: A version of 304 stabilized with titanium to prevent carbide precipitation during welding. It has a slightly higher strength than 304L and is more suitable for high-temperature use.
- Type 347: Stabilized with niobium.
- Type 316: In this alloy, molybdenum is added to improve the corrosion resistance in reducing conditions, such as in dilute sulfuric acid, and, in particular, to solutions containing chlorides.
- Type 316L: A low-carbon version of type 316, which should be specified if welding or heat treatment is liable to cause carbide precipitation in type 316.
- Types 309/310: Alloys with a high chromium content to give greater resistance to oxidation at high temperatures. Alloys with greater than 25% Cr are susceptible to embrittlement due to sigma phase formation at temperatures above 500 °C. Sigma phase is an intermetallic compound, FeCr. The formation of the sigma phase in austenitic stainless steels is discussed by Hills and Harries (1960).

Mechanical properties

The austenitic stainless steels have greater strength than the plain carbon steels, particularly at elevated temperatures (Table 6.7).

As was mentioned in Section 6.3.7, the austenitic stainless steels, unlike the plain carbon steels, do not become brittle at low temperatures. It should be noted that the thermal conductivity of stainless steel is significantly lower than that of mild steel.

TABLE 6.7 Comparative strength of carbon steel and stainless steel

Temperature °F		100	300	500	700	900
Maximum allowable stress (1000 psi)	Carbon steel (A285 plate)	12.9	12.9	12.9	11.5	5.9
	Stainless steel (304L plate)	16.7	16.7	14.7	13.5	11.9

Maximum allowable stress values from ASME BPV Code Sec. II Part D.

Typical values at 100 °C are:	**type 304 (18/8)**	**mild steel**
	16 W/m°C	60 W/m°C

Austenitic stainless steels are nonmagnetic in the annealed condition.

General corrosion resistance

The higher the alloying content, the better the corrosion resistance over a wide range of conditions, strongly oxidizing to reducing, but with a higher cost. A ranking in order of increasing corrosion resistance, taking type 304 as 1, is given here:

304	304L	321	316	316L	310
1.0	1.1	1.1	1.25	1.3	1.6

Intergranular corrosion (weld decay) and stress corrosion cracking are problems associated with the use of stainless steels and must be considered when selecting types suitable for use in a particular environment. Stress corrosion cracking in stainless steels can be caused by a few parts per million (ppm) of chloride ions (see Section 6.4.5).

In general, stainless steels are used for corrosion resistance when oxidizing conditions exist. Special types, or other high-nickel alloys, should be specified if reducing conditions are likely to occur. The properties, corrosion resistance, and uses of the various grades of stainless steel are discussed fully by Peckner and Bernstein (1977). A comprehensive discussion of the corrosion resistance of stainless steels is given in Sedriks (1996). Stress corrosion cracking in stainless steels is discussed by Turner (1989).

High-alloy-content stainless steels

Super-austenitic, high-nickel stainless steels, containing between 29% and 30% nickel and 20% chromium, have a good resistance to acids and acid chlorides. They are more expensive than the lower-alloy content, 300 series, of austenitic stainless steels.

Duplex and super-duplex stainless steels contain high percentages of chromium. They are called *duplex* because their structure is a mixture of the austenitic and ferritic phases. They have better corrosion resistance than the austenitic stainless steels and are less susceptible to stress corrosion cracking. The chromium content of duplex stainless steels is around 20%, and around 25% in the super-duplex grades. The super-duplex steels were developed for use in aggressive offshore environments.

The duplex range of stainless steels can be readily cast, wrought, and machined. Problems can occur in welding as a result of the need to keep the correct balance of ferrite and austenite in the weld area, but this can be overcome using the correct welding materials and procedures.

The cost of the duplex grades is comparable with the 316 steels. Super-duplex is around 50% higher than the cost of duplex.

The selection and properties of duplex stainless steels are discussed by Bendall and Guha (1990), and Warde (1991).

6.8.3 Nickel

Nickel has good mechanical properties and is easily worked. The pure metal (>99%) is not generally used for chemical plants; instead, its alloys are preferred for most applications. The main use is for equipment handling

caustic alkalis at temperatures above that at which carbon steel could be used: above 70 °C. Nickel is not subject to corrosion cracking like stainless steel.

6.8.4 Monel

Monel, the classic nickel–copper alloy with the metals in the ratio 2:1, is probably, after the stainless steels, the most commonly used alloy for chemical plants. It is easily worked and has good mechanical properties up to 500 °C. It is more expensive than stainless steel but is not susceptible to stress-corrosion cracking in chloride solutions. Monel has good resistance to dilute mineral acids and can be used in reducing conditions, where the stainless steels would be unsuitable. It may be used for equipment handling alkalis, organic acids and salts, and sea water.

6.8.5 Inconel and Incoloy

Inconel (typically 76% Ni, 7% Fe, 15% Cr) is used primarily for acid resistance at high temperatures. It maintains its strength at elevated temperature and is resistant to furnace gases, if sulfur-free. It is not suitable for use in sulfidizing environments. Nickel alloys with higher chromium content such as Incoloy 800 (21% Cr) and RA-33 (25% Cr) have better oxidation resistance at higher temperatures.

6.8.6 The Hastelloys

The trade name Hastelloy covers a range of nickel, chromium, molybdenum, and iron alloys that were developed for corrosion resistance to strong mineral acids, particularly HCl. The corrosion resistance, and use, of the two main grades, Hastelloy B (65% Ni, 28% Mo, 6% Fe) and Hastelloy C (54% Ni, 17% Mo, 15% Cr, 5% Fe), are discussed in papers by Weisert (1952a,b).

6.8.7 Copper and copper alloys

Pure copper is not widely used for chemical equipment. It has been used traditionally in the food industry, particularly in brewing. Copper is a relatively soft, very easily worked metal, and is used extensively for small-bore pipes and tubes.

The main alloys of copper are the brasses, alloyed with zinc, and the bronzes, alloyed with tin. Other so-called bronzes are the aluminum bronzes and the silicon bronzes.

Copper is attacked by mineral acids except cold, dilute, unaerated sulfuric acid. It is resistant to caustic alkalis, except ammonia, and to many organic acids and salts. The brasses and bronzes have a similar corrosion resistance to the pure metal. Their main use in the chemical industry is for valves and other small fittings and for heat exchanger tubes and tube sheets. If brass is used, a grade must be selected that is resistant to dezincification.

The cupro–nickel alloys (70% Cu) have good resistance to corrosion-erosion and are used for heat exchanger tubes, particularly where sea water is used as a coolant.

6.8.8 Aluminum and its alloys

Pure aluminum lacks mechanical strength but has higher resistance to corrosion than its alloys. The main structural alloys used are the Duralumin (Dural) range of aluminum–copper alloys (typical composition 4% Cu, with 0.5% Mg), which have a tensile strength equivalent to that of mild steel. The pure metal can be used as a cladding on Dural plates to combine the corrosion resistance of the pure metal with the strength of the alloy. The corrosion resistance of aluminum is due to the formation of a thin oxide film (as with the stainless steels). It is therefore most suitable for use in strong oxidizing conditions. It is attacked by mineral acids and by alkalis but is suitable for concentrated nitric acid (greater than 80%). It is widely used in the textile and food industries, where the use of mild steel would cause contamination. It is also used for the storage and distribution of demineralized water.

6.8.9 Lead

Lead was one of the traditional materials of construction for chemical plants but has now, because of its price, been largely replaced by other materials, particularly plastics. It is a soft, ductile material and is mainly used in the form of sheets (as linings) or pipe. It has a good resistance to acids, particularly sulfuric.

6.8.10 Titanium

Titanium is now used quite widely in the chemical industry, mainly for its resistance to halide solutions, including sea water and wet chlorine. It is rapidly attacked by dry chlorine, but the presence of as low a concentration of moisture as 0.01% will prevent attack. Like the stainless steels, titanium depends for its resistance on the formation of an oxide film. Titanium is also used in other halide services, for example, in liquid phase oxidation processes, such as the manufacture of terephthalic acid, that use bromide as a catalyst or promoter.

Alloying with palladium (0.15%) significantly improves the corrosion resistance, particularly to HCl. Titanium is being increasingly used for heat exchangers, replacing cupro–nickel for use with sea water.

The use of titanium for corrosion resistance is discussed by Deily (1997).

6.8.11 Tantalum

The corrosion resistance of tantalum is similar to that of glass, and it has been called a *metallic* glass. It is expensive, about five times the cost of stainless steel, and is used for special applications, where glass or a glass lining would not be suitable. Tantalum plugs are used to repair glass-lined equipment.

The use of tantalum as a material of construction in the chemical industry is discussed by Fensom and Clark (1984) and Rowe (1994, 1999).

6.8.12 Zirconium

Zirconium and zirconium alloys are used in the nuclear industry because of their low neutron absorption cross-section and resistance to hot water at high pressures.

In the chemical industry zirconium is finding use where resistance to hot and boiling acids is required: nitric, sulfuric, and particularly hydrochloric. Its resistance is equivalent to that of tantalum, but zirconium is less expensive, similar in price to high-nickel steel. Rowe (1999) gives a brief review of the properties and use of zirconium for chemical plants.

6.8.13 Silver

Silver linings are used for vessels and equipment handling hydrofluoric acid. It is also used for special applications in the food and pharmaceutical industries, where it is vital to avoid contamination of the product.

6.8.14 Gold

Because of its high cost, gold is rarely used as a material of construction. It is highly resistant to attack by dilute nitric acid and hot concentrated sulfuric acid, but is dissolved by aqua regia (a mixture of concentrated nitric and sulfuric acids). It is attacked by chlorine and bromine, and forms an amalgam with mercury. It has been used as thin plating on condenser tubes and other surfaces.

6.8.15 Platinum

Platinum has a high resistance to oxidation at high temperatures. One of its main uses has been in the form of an alloy with copper in the manufacture of the spinnerets used in synthetic textile spinning processes.

6.9 Plastics as materials of construction for chemical plants

Plastics are being increasingly used as corrosion-resistant materials for chemical plant construction. They are also widely used in food processing and biochemical plants. They can be divided into two broad classes:

1. Thermoplastic materials, which soften with increasing temperature, for example, polyvinyl chloride (PVC) and polyethylene
2. Thermosetting materials, which have a rigid, cross-linked structure, for example, the polyester and epoxy resins

Details of the chemical composition and properties of the wide range of plastics used as engineering material can be found in the books by Butt and Wright (1980), Evans (1980), and Harper (2001).

The biggest use of plastics is for piping; sheets are also used for lining vessels and for fabricated ducting and fan casings. Moldings are used for small items, such as pump impellers, valve parts, and pipe fittings.

The mechanical strength and operating temperature of plastics are low compared with metals. The mechanical strength, and other properties, can be modified by the addition of fillers and plasticizers. When reinforced with glass or carbon fibers, thermosetting plastics can have a strength equivalent to mild steel at low temperatures and are used for pressure vessels and pressure piping. Guidelines for the design of fiber-reinforced plastic pressure vessels are given in the ASME BPV Code Sec. X Part RD. Unlike metals, plastics are flammable. Plastics can be considered to complement metals as corrosion-resistant materials of construction. They generally have good resistance to dilute acids and inorganic salts, but suffer degradation in organic solvents that would not attack metals. Unlike metals, plastics can absorb solvents, causing swelling and softening. The properties and typical areas of use of the main plastics used for chemical plants are reviewed briefly in the following sections. A comprehensive discussion of the use of plastics as corrosion-resistant materials is given in a book by Fontana (1986). Information on the selection of plastics for different applications is also given by Harper (2001). The mechanical properties and relative cost of plastics are given in Table 6.8.

6.9.1 Polyvinyl chloride

PVC is probably the most commonly used thermoplastic material in the chemical industry. Of the available grades, rigid (unplasticized) PVC is the most widely used. It is resistant to most inorganic acids, except strong sulfuric and nitric acids, and inorganic salt solutions. It is unsuitable, because of swelling, for use with most organic solvents. The maximum operating temperature for PVC is low: 60 °C. The use of PVC as a material of construction in chemical engineering is discussed in a series of articles by Mottram and Lever (1957).

6.9.2 Polyolefins

Low-density polyethylene is a relatively cheap, tough, flexible plastic. It has a low softening point and is not suitable for use above about 60 °C. The higher-density polymer (950 kg/m^3) is stiffer and can be used at higher temperatures. Polypropylene is a stronger material than the polyethylenes and can be used at temperatures up to 120 °C. The chemical resistance of the polyolefins is similar to that of PVC.

6.9.3 Polytetrafluoroethylene

Polytetrafluoroethylene (PTFE), known under the trade names Teflon and Fluon, is resistant to all chemicals except molten alkalis and fluorine, and can be used at temperatures up to 250 °C. It is a relatively weak material, but its mechanical strength can be improved by the addition of fillers (glass and carbon fibers). It is expensive and difficult to fabricate. PTFE is used extensively for gaskets, gland packings (for example, on valve stems), and demister pads. As a coating, it is used to confer nonstick properties to surfaces such as filter plates. It can also be used as a liner for vessels.

TABLE 6.8 Mechanical properties and relative cost of polymers

Material	Tensile strength (N/mm^2)	Elastic modulus (kN/mm^2)	Density (kg/m^3)	Relative cost
PVC	55	3.5	1400	1.5
Polyethylene (low density)	12	0.2	900	1.0
Polypropylene	35	1.5	900	1.5
PTFE	21	1.0	2100	30.0
GRP polyester	100	7.0	1500	3.0
GRP epoxy	250	14.0	1800	5.0

Approximate cost relative to polyethylene, volumetric basis.

6.9.4 Polyvinylidene fluoride

Polyvinylidene fluoride (PVDF) has properties similar to PTFE but is easier to fabricate. It has good resistance to inorganic acids and alkalis and organic solvents. It is limited to a maximum operating temperature of 140 °C.

6.9.5 Glass-fiber–reinforced plastics

The polyester resins, reinforced with glass fiber, are the most common thermosetting plastics used for chemical plants. Complex shapes can be easily formed using the techniques developed for working with reinforced plastics. Glass-reinforced plastics are relatively strong and have a good resistance to a wide range of chemicals. The mechanical strength depends on the resin used, the form of the reinforcement (chopped mat or cloth), and the ratio of resin to glass.

By using special techniques, in which the reinforcing glass fibers are wound on in the form of a continuous filament, high strength can be obtained, and this method is used to produce pressure vessels.

The polyester resins are resistant to dilute mineral acids, inorganic salts, and many solvents. They are less resistant to alkalis.

Glass-fiber–reinforced epoxy resins are also used for chemical plants but are more expensive than the polyester resins. In general they are resistant to the same range of chemicals as the polyesters, but are more resistant to alkalis.

The chemical resistance of glass-fiber–reinforced plastic (GRP) is dependent on the amount of glass reinforcement used. High ratios of glass to resin give higher mechanical strength but generally lower resistance to some chemicals. The design of chemical plant equipment in GRP is the subject of a book by Malleson (1969); see also Shaddock (1971), Baines (1984), and ASME BPV Code Sec. X.

6.9.6 Rubber

Rubber, particularly in the form of linings for tanks and pipes, has been extensively used in the chemical industry for many years. Natural rubber is most commonly used because of its good resistance to acids (except concentrated nitric acid) and alkalis. It is unsuitable for use with most organic solvents.

Synthetic rubbers are also used for particular applications. Hypalon (trademark, E. I. du Pont de Nemours) has a good resistance to strongly oxidizing chemicals and can be used with nitric acid. It is unsuitable for use with chlorinated solvents. Viton (trademark, E. I. du Pont de Nemours) has a better resistance to solvents, including chlorinated solvents, than other rubbers. Both Hypalon and Viton are expensive compared with other synthetic and natural rubbers.

The use of natural rubber lining is discussed by Saxman (1965) and the chemical resistance of synthetic rubbers by Evans (1963). Butt and Wright (1984) give an authoritative account of the application and uses of rubber and plastic linings and coatings.

6.10 Ceramic materials (silicate materials)

Ceramics are compounds of nonmetallic elements and include the following materials used for chemical plants:

- Glass, the borosilicate glasses (hard glass)
- Stoneware
- Acid-resistant bricks and tiles
- Refractory materials
- Cements and concrete
- Ceramic materials have a cross-linked structure and are therefore brittle.

6.10.1 Glass

Borosilicate glass (known by several trade names, including Pyrex) is used for chemical plants as it is stronger than the soda glass used for general purposes; it is more resistant to thermal shock and chemical attack. Glass equipment is often used in small-scale manufacture of specialty chemicals. Glass can be used up to moderately high temperatures (700 °C) but is not suitable for pressures above atmospheric unless used as a lining.

Glass equipment is available from several specialist manufacturers. Pipes and fittings are produced in a range of sizes, up to 0.5 m. Special equipment, such as heat exchangers, is available and, together with the larger sizes of pipe, can be used to construct distillation and absorption columns. Teflon gaskets are normally used for jointing glass equipment and pipes.

Where failure of the glass could cause injury, pipes and equipment should be protected by external shielding or wrapping with plastic tape. Glass apparatus should allow adequate venting to the atmosphere to handle anticipated relief scenarios without accumulating high pressure.

Glass linings, also known as *glass enamel*, have been used on steel and iron vessels for many years. Borosilicate glass is used, and the thickness of the lining is about 1 mm. The techniques used for glass lining, and the precautions to be taken in the design and fabrication of vessels to ensure a satisfactory lining, are discussed by Landels and Stout (1970) and by the ASME BPV Code Sec. VIII Div. 1, Mandatory Appendix 27. Borosilicate glass is resistant to acids, salts, and organic chemicals. It is attacked by the caustic alkalis and fluorine.

6.10.2 Stoneware

Chemical stoneware is similar to the domestic variety, but of higher quality, stronger, and with a better glaze. It is available in a variety of shapes for pipe runs and columns. As for glass, it is resistant to most chemicals except alkalis and fluorine. The composition and properties of chemical stoneware are discussed by Holdridge (1961). Stoneware and porcelain shapes are used for packing absorption and distillation columns (see Chapter 17).

6.10.3 Acid-resistant bricks and tiles

High-quality bricks and tiles are used for lining vessels and ditches and to cover floors. The linings are usually backed with a corrosion-resistant membrane of rubber or plastic, placed behind the tiles, and special acid-resistant cements are used for the joints. Brick and tile linings are covered in a book by Falcke and Lorentz (1985).

6.10.4 Refractory materials (refractories)

Refractory bricks and cements are needed for equipment operating at high temperatures, such as fired heaters, high-temperature reactors, and boilers. The refractory bricks in common use are composed of mixtures of silica (SiO_2) and alumina (Al_2O_3). The quality of the bricks is largely determined by the relative amounts of these materials and the firing temperature. Mixtures of silica and alumina form a eutectic composition (94.5% SiO_2, 1545 °C), and for a high refractoriness under load (the ability to resist distortion at high temperature), the composition must be well removed from the eutectic composition. The highest-quality refractory bricks, for use in load-bearing structures at high temperatures, contain high proportions of silica or alumina. "Silica bricks," containing greater than 98% SiO_2, are used for general furnace construction. High-alumina bricks, 60% Al_2O_3, are used for special furnaces where resistance to attack by alkalis is important, such as lime and cement kilns. Fire bricks, typical composition 50% SiO_2, 40% Al_2O_3, and the balance CaO and Fe_2O_3, are used for general furnace construction. Silica can exist in a variety of allotropic forms, and bricks containing a high proportion of silica undergo reversible expansion when heated up to working temperature. The higher the silica content, the greater the expansion, and this must be allowed for in furnace design and operation.

Ordinary fire bricks, fire bricks with a high porosity, and special bricks composed of diatomaceous earths are used for insulating walls.

Full details of the refractory materials used for process and metallurgical furnaces can be found in the books by Norton (1968) and Lyle (1947). Additional information on refractories can be found in the books by Schacht (1995, 2004) and Routschka and Wuthnow (2008).

6.11 Carbon

Impervious carbon, impregnated with chemically resistant resins, is used for specialized equipment, particularly heat exchangers. It has high conductivity and good resistance to most chemicals, except oxidizing acids of concentrations greater than 30%. Carbon tubes can be used in conventional shell and tube exchanger arrangements, or

proprietary designs can be used, in which the fluid channels are formed in blocks of carbon; see Hilland (1960) and Denyer (1991).

6.12 Protective coatings

A wide range of paints and other organic coatings is used for the protection of mild steel structures. Paints are used mainly for protection from atmospheric corrosion. Special chemically resistant paints have been developed for use on chemical process equipment. Chlorinated rubber paints and epoxy-based paints are used. In the application of paints and other coatings, good surface preparation is essential to ensure good adhesion of the paint film or coating.

Brief reviews of the paints used to protect chemical plants are given by Ruff (1984) and Hullcoop (1984).

6.13 Design for corrosion resistance

The life of equipment subjected to corrosive environments can be increased by proper attention to design details. Equipment should be designed to drain freely and completely. The internal surfaces should be smooth and free from crevices where corrosion products and other solids can accumulate. Butt joints should be used in preference to lap joints. The use of dissimilar metals in contact should be avoided, or care taken to ensure that they are effectively insulated to avoid galvanic corrosion. Fluid velocities and turbulence should be high enough to avoid the deposition of solids but not so high as to cause erosion-corrosion. The design and operating procedures should make allowance for changes in the environment to which the materials are exposed. For example, heating and cooling rates should be slow enough to prevent thermal shocks, and care should be taken during maintenance not to damage corrosion-resistant films that have developed during operation.

6.14 References

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6.15 Nomenclature

		Dimensions in MLT$
A	Area	$\mathbf{L^2}$
C	Cost of material	$\mathbf{\$/M}$
t	Time	$\mathbf{T}$
w	Mass loss	$\mathbf{M}$
P	Density	$\mathbf{ML^{-3}}$
σ_d	Maximum allowable stress	$\mathbf{ML^{-1}\,T^{-2}}$

6.16 Problems

6.1. A pipeline constructed of carbon steel failed after 3 years of operation. On examination it was found that the wall thickness had been reduced by corrosion to about half the original value. The pipeline was constructed of nominal 100 mm (4 in) schedule 40, pipe, inside diameter 102.3 mm (4.026 in), and outside diameter 114.3 mm (4.5 in). Estimate the rate of corrosion in ipy and mm per year.

6.2. The pipeline described in Question 6.1 was used to carry wastewater to a hold-up tank. The effluent is not hazardous. A decision has to be made on what material to use to replace the pipe. Three suggestions have been made:

1. Replace with the same schedule carbon steel pipe and accept renewal at 3-year intervals.
2. Replace with a thicker pipe, schedule 80, outside diameter 114.3 mm (4.5 in) and inside diameter 97.2 mm (3.826 in).
3. Use stainless steel pipe, which will not corrode.

The estimated cost of the pipes per unit length is schedule 40 carbon steel $5, schedule 80 carbon steel $8.3, and stainless steel (304) schedule 40 $24.8.

- Installation and fittings for all the materials add $16.5 per unit length.
- The downtime required to replace the pipe does not result in a loss of production.
- If the expected future life of the plant is 7 years, recommend which pipe to use.

6.3. Choose a suitable material of construction for the following duties:

1. 98% w/w sulfuric acid at 70 °C.
2. 5% w/w sulfuric acid at 30 °C.
3. 30% w/w hydrochloric acid at 50 °C.
4. 5% aqueous sodium hydroxide solution at 30 °C.
5. Concentrated aqueous sodium hydroxide solution at 50 °C.
6. 5% w/w nitric acid at 30 °C.
7. Boiling concentrated nitric acid.
8. 10% w/w sodium chloride solution.
9. A 5% w/w solution of cuprous chloride in hydrochloric acid.
10. 10% w/w hydrofluoric acid.

In each case, select the material for a 50-mm pipe operating at approximately 2 bar pressure.

6.4. Suggest suitable materials of construction for the following applications:

1. A 10,000 m^3 storage tank for toluene.
2. A 5.0 m^3 tank for storing a 30% w/w aqueous solution of sodium chloride.
3. A 2 m diameter, 20 m high distillation column, distilling acrylonitrile.
4. A 100 m^3 storage tank for strong nitric acid.
5. A 500 m^3 aqueous waste hold-up tank. The wastewater pH can vary from 1 to 12. The wastewater will also contain traces of organic material.
6. A packed absorption column 0.5 m diameter, 3 m high, absorbing gaseous hydrochloric acid into water. The column will operate at essentially atmospheric pressure.

6.5. Aniline is manufactured by the hydrogenation of nitrobenzene in a fluidized bed reactor. The reactor operates at 250 °C and 20 bar. The reactor vessel is approximately 3 m diameter and 9 m high. Suggest suitable materials of construction for this reactor.

6.6. Methyl ethyl ketone (MEK) is manufactured by the dehydrogenation of 2-butanol using a shell and tube type reactor. Flue gases are used for heating and pass though the tubes. The flue gases will contain traces of sulfur dioxide. The reaction products include hydrogen.
The reaction takes place in the shell at a pressure of 3 bar and temperature of 500 °C. Select suitable materials for the tubes and shell.

6.7. In the manufacture of aniline by the hydrogenation of nitrobenzene, the off-gases from the reactor are cooled and the products and unreacted nitrobenzene condensed in a shell and tube exchanger. A typical composition of the condensate is kmol/h: aniline 950, cyclo-hexylamine 10, water 1920, nitrobenzene 40. The gases enter the condenser at 230 °C and leave at 50 °C. The cooling water enters the tubes at 20 °C and leaves at 50 °C. Suggest suitable materials of construction for the shell and the tubes.

6.8. A slurry of acrylic polymer particles in water is held in storage tanks before filtering and drying. Plain carbon steel would be a suitable material for the tanks, but it is essential that the polymer does not become contaminated with iron in storage. Suggest some alternative materials of construction for the tanks.

6.9. Coal gasification is carried out at 850 °C and 40 atmospheres pressure by reaction of coal with steam and oxygen. The empirical formula of the coal is roughly $CH_{0.8}S_{0.013}$. What materials of construction would you recommend for:

- The coal addition system
- The oxygen injection system
- The gasification reactor
- The product gas transfer line

CHAPTER

7

Capital cost estimating

KEY LEARNING OBJECTIVES

- Techniques for estimating the capital cost of a process
- How to estimate the costs of major process equipment
- How to use commercial cost estimating software
- How to update cost data
- How to estimate cost data for international projects
- How to estimate costs for proprietary equipment when data are scarce

7.1 Introduction

Most chemical engineering design projects are carried out to provide information from which estimates of capital and operating costs can be made. Chemical plants are built to make a profit, and an estimate of the investment required is needed before the profitability of a project can be assessed. Cost estimation is a specialized subject and a profession in its own right, but the design engineer must be able to make rough cost estimates to decide between project alternatives and optimize the design.

This chapter introduces the components of capital costs and the techniques used for capital cost estimating. Simple costing methods and some cost data are given, which can be used to make preliminary estimates of capital costs in the early stages of design. Sources of cost data and methods for updating cost estimates are described. The more sophisticated software that is used in industry for preliminary estimating is discussed in Section 7.10.

For a more detailed treatment of the subject, the reader should refer to the numerous specialized texts that have been published on cost estimation. The following books are particularly recommended: Happle and Jordan (1975), Guthrie (1974), Page (1996), Garrett (1989), Humphreys (1991, 2005).

7.2 Components of capital cost

This section introduces the components of project costs.

7.2.1 Fixed capital investment

The fixed capital investment is the total cost of designing, constructing, and installing a plant and the associated modifications needed to prepare the plant site. The fixed capital investment is made up of:

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1. The inside battery limits (ISBL) investment − the cost of the plant itself
2. The modifications and improvements that must be made to the site infrastructure, known as *offsite battery limits* (OSBL) investment
3. Engineering and construction costs
4. Contingency charges

ISBL plant costs

The ISBL plant cost includes the cost of procuring and installing all the process equipment that makes up the new plant.

The direct field costs include:

1. All the major process equipment, such as vessels, reactors, columns, furnaces, heat exchangers, coolers, pumps, compressors, motors, fans, turbines, filters, centrifuges, driers, etc., including field fabrication and testing if necessary.
2. Bulk items, such as piping, valves, wiring, instruments, structures, insulation, paint, lube oils, solvents, catalysts, etc.
3. Civil works such as roads, foundations, piling, buildings, sewers, ditches, bunds, etc.
4. Installation labor and supervision.

In addition to the direct field costs there will be indirect field costs, including:

1. Construction costs such as construction equipment rental, temporary construction (rigging, trailers, etc.), temporary water and power, construction workshops, etc.
2. Field expenses and services such as field canteens, specialists' costs, overtime pay, and adverse weather costs.
3. Construction insurance.
4. Labor benefits and burdens (social security, workers compensation, etc.).
5. Miscellaneous overhead items such as agent's fees, legal costs, import duties, special freight costs, local taxes, patent fees or royalties, corporate overheads, etc.

In the early stages of a project it is important to define the ISBL scope carefully, as other project costs are often estimated from ISBL cost. The overall project economics can be badly miscalculated if the ISBL scope is poorly defined. Several methods for estimating ISBL costs are given in the following sections of this chapter.

Offsite costs

Offsite cost or OSBL investment includes the costs of the additions that must be made to the site infrastructure to accommodate adding a new plant or increasing the capacity of an existing plant. Offsite investments may include:

- Electric main substations, transformers, switchgear, and power lines
- Power generation plants, turbine engines, and standby generators
- Boilers, steam mains, condensate lines, boiler feed water treatment plant, and supply pumps
- Cooling towers, circulation pumps, cooling water mains, and cooling water treatment
- Water pipes, water demineralization, waste water treatment plant, site drainage, and sewers
- Air separation plants to provide site nitrogen for inert gas, as well as nitrogen lines
- Driers and blowers for instrument air, as well as instrument air lines
- Pipe bridges, feed, and product pipelines
- Tanker farms, loading facilities, silos, conveyors, docks, warehouses, railroads, and lift trucks
- Laboratories and analytical equipment
- Offices, canteens, changing rooms, and central control rooms
- Workshops and maintenance facilities
- Emergency services, firefighting equipment, fire hydrants, medical facilities, etc.
- Site security, fencing, gatehouses, and landscaping

Offsite investments often involve interactions with utility companies such as electricity or water suppliers. They may be subject to equal or greater scrutiny than ISBL investments because of their impact on the local community through water consumption and discharge, traffic, and other similar factors.

Offsite costs are typically estimated as a proportion of ISBL costs in the early stages of design. Offsite costs are usually in the range from 10% to 100% of ISBL costs, depending on the project scope and its impact on site infrastructure. For typical petrochemical projects, offsite costs are usually between 20% and 50% of ISBL cost, and 40% is usually used as an initial estimate if no details of the site are known. For an established site with well-developed

infrastructure, offsite costs will generally be lower. This is particularly true of sites that have undergone contraction, where some plants have closed, leaving underutilized infrastructure ("brownfield" sites). On the other hand, if the site infrastructure is in need of repair or upgrading to meet new regulations, or if the plant is built on a completely new site (a "greenfield" site), then offsite costs will be higher. Offsite costs are discussed in more detail in Section 7.9.

Once a site has been chosen for the project, the modifications to the site infrastructure that are needed can be designed in detail in the same manner as the ISBL investments. Infrastructure upgrades are usually the first part of a project to be implemented, as they usually need to be commissioned before the plant can begin operation.

Engineering costs

The engineering costs, sometimes referred to as *home office costs* or *contractor charges,* include the costs of detailed design and other engineering services required to carry out the project:

1. Detailed design engineering of process equipment, piping systems, control systems and offsites, plant layout, drafting, cost engineering, scale models, and civil engineering.
2. Procurement of main plant items and bulks.
3. Construction supervision and services.
4. Administrative charges, including engineering supervision, project management, expediting, inspection, travel and living expenses, and home office overheads.
5. Bonding.
6. Contractor's profit.

Very few operating companies retain a large enough engineering staff to carry out all of these activities internally, except for very small projects. In most cases, one or more of the major engineering contracting firms will be brought in.

Engineering costs are best estimated individually based on project scope, as they are not directly proportional to project size. A rule of thumb for engineering costs is 30% of ISBL plus OSBL cost for smaller projects and 10% of ISBL plus OSBL cost for larger projects. The actual charges paid for real industrial projects vary considerably from customer to customer and are strongly influenced by long-term client−contractor relationships and overall market demand for engineering services. Customers usually have to pay premiums or surcharges if they want to complete a project on an accelerated timeline or if they make a lot of changes once a project is underway.

Contingency charges

Contingency charges are extra costs added into the project budget to allow for variation from the cost estimate. All cost estimates are uncertain (see Section 7.3.1), and the final installed cost of many items is not known until installation has been successfully completed. Apart from errors in the cost estimate, contingency costs also help cover:

- Minor changes in project scope
- Changes in prices (e.g., prices of steel, copper, catalyst, etc.)
- Currency fluctuations
- Labor disputes
- Subcontractor problems
- Other unexpected problems

A contingency charge can be thought of as an additional fee charged by the Engineering, Procurement and Construction (EPC) company to address the risk that the project will run over budget. Contingency charges therefore reduce the likelihood that the contractor will lose money on a fixed-price bid. A minimum contingency charge of 10% of ISBL plus OSBL cost should be used on all projects. If the technology is uncertain, higher contingency charges (up to 50%) are used. Contingency charges are discussed in more detail in Section 9.8.4.

7.2.2 Working capital

In addition to the fixed capital investment that was used to design and construct the plant, the owner needs to invest some capital in maintaining plant operations. The capital that is tied up in maintaining inventories of feeds, products, and spare parts, together with cash on hand and the difference between money owed by costumers (accounts receivable) and money owed to suppliers (accounts payable), is termed the *working capital* of the plant. Working capital is required as long as the plant is in operation, but is recovered if the plant is shut down. Working capital is discussed in more detail in the chapter on project finance and economics; see Section 9.2.3.

7.3 Accuracy and purpose of capital cost estimates

The accuracy of an estimate depends on the amount of design detail available, the accuracy of the cost data available, and the time spent on preparing the estimate. In the early stages of a project only an approximate estimate will be justified based on the amount of information available.

7.3.1 AACE International cost estimate classes

The Association for the Advancement of Cost Estimating International (AACE International) is the professional association representing the cost engineering profession in the United States. AACE International classifies capital cost estimates into five types according to their accuracy and purpose:

1. Order of magnitude estimates ("ballpark estimate," "guesstimate" "Class 5 estimate"), accuracy typically ±30% to 50%, usually based on the costs of similar processes and requiring essentially no design information. These are used in initial feasibility studies and for screening purposes.
2. Preliminary ("approximate," "study," "feasibility," "Class 4") estimates, accuracy typically ±30%, which are used to make coarse choices between design alternatives. They are based on limited cost data and design detail.
3. Definitive ("authorization," "budgeting," "control," "Class 3") estimates, accuracy typically ±10% to 15%. These are used for the authorization of funds to proceed with the design to the point where an accurate and more detailed estimate can be made. Authorization may also include funds to cover cancellation charges on any long delivery equipment ordered at this stage of the design to avoid delay in the project. In a contracting organization this type of estimate could be used with a large contingency factor to obtain a price for tendering a bid. Normally, however, an accuracy of about ±5% would be needed and a more detailed estimate would be made if time permitted. With experience, and where a company has cost data available from similar projects, estimates of acceptable accuracy can be made at the flowsheet stage of the project. A rough P&I diagram and the approximate sizes of the major items of equipment would also be needed.
4. Detailed estimates ("quotation," "tender," "firm estimate," "contractor's estimate," "Class 2 estimate"), accuracy ±5% to 10%, which are used for project cost control and estimates for fixed-price contracts. Estimates of this quality can be made once the front-end engineering design (FEED) is completed, including a complete (or near-complete) process design, firm quotes for equipment, and a detailed breakdown and estimation of the construction cost. By this stage, the contractor can usually present a list of all the items that must be purchased and can make a firm commitment to the client.
5. Check estimates ("tender," "as-bid," "Class 1 estimate"), accuracy ±5% to 10%. This is based on a completed design and concluded negotiations on procurement of specialized items and long lead-time items.

It is important for design engineers to understand how much information is necessary to arrive at a given level of confidence in an estimate, particularly when working with professional cost engineers. It is not possible to generate a Class 1 or Class 2 estimate without completing the design to a sufficient level of detail. A Class 3 estimate may also require a substantially complete design package unless the company has recently built projects with similar scope. Class 4 and 5 estimates are relatively easy to generate but have high uncertainty, which must be taken into consideration in economic analysis and sensitivity analysis; see Section 9.8.

7.3.2 Development of cost estimates

As a project proceeds from initial concept through detailed design to start-up, costs begin to be accumulated, particularly once procurement and construction get underway (Fig. 7.1a). At the same time, the ability of the design engineer to influence project cost decreases and is minimal by the time construction begins (Fig. 7.1b). There is therefore a strong incentive to try to estimate project costs at as early a stage as possible, even if the design information is incomplete, so that the project can be optimized, evaluated, and abandoned if it is not attractive.

It is difficult to go beyond the accuracy of a Class 4 estimate without making a fairly detailed design of the plant. The cost of preparing the estimate thus becomes the cost of designing the process and sizing and optimizing the main equipment items. To obtain even greater accuracy, the contractor needs to establish the plot plan and plant layout so as to make more accurate estimates of the amount of piping, wiring, and structural steel that will be needed. The cost of preparing an estimate thus increases from about 0.1% of the total project cost for ±30% accuracy to about 3% for a detailed estimate with an accuracy of ±5%.

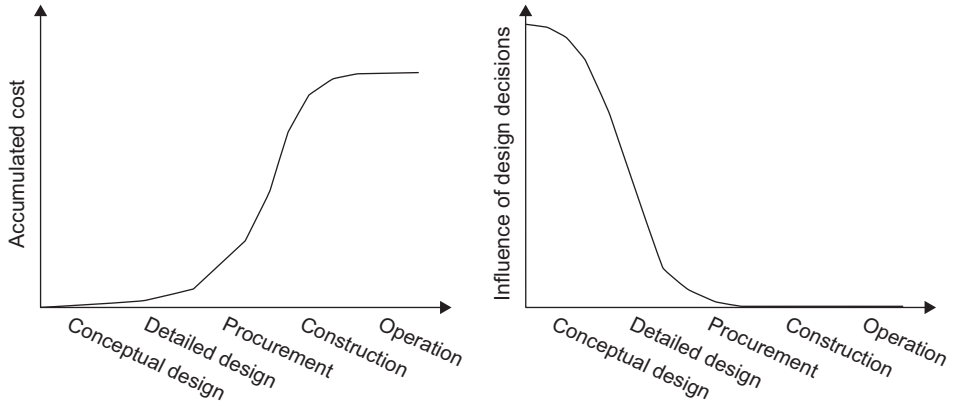


FIG. 7.1 Influence of design decisions on project cost.

7.4 Order-of-magnitude estimates

In the early stages of design, or when carrying out preliminary marketing studies, the design engineer may want to make a quick (Class 5) capital cost estimate without completing a plant design. Several shortcut methods have been developed that allow estimates of total plant cost to be made within ±50% accuracy for preliminary studies. These methods can also be used to provide a rough check on more detailed estimates developed from process equipment costs later in the design of the process.

7.4.1 Cost curve methods

The quickest way to make an order-of-magnitude estimate of plant cost is to scale it from the known cost of an earlier plant that used the same technology or from published data. This requires no design information other than the production rate.

The capital cost of a plant can be related to capacity by the equation

$$C_2 = C_1 \left(\frac{S_2}{S_1}\right)^n \tag{7.1}$$

where C_2 = ISBL capital cost of the plant with capacity S_2
C_1 = ISBL capital cost of the plant with capacity S_1

The exponent n is typically 0.8 to 0.9 for processes that use a lot of mechanical work or gas compression (e.g., methanol, paper pulping, solids-handling plants). For typical petrochemical processes n is usually about 0.7. For small-scale, highly instrumented processes, such as specialty chemical or pharmaceuticals manufacture, n is in the range of 0.4 to 0.5. Averaged across the whole chemical industry, n is about 0.6, and hence Equation 7.1 is commonly referred to as the *six-tenths rule*. The equation can be used with $n = 0.6$ to get a rough estimate of the capital cost if there are not sufficient data available to calculate the index for the particular process. Estrup (1972) gives a critical review of the six-tenths rule. Equation 7.1 is only an approximation, and if sufficient data are available, the relationship is best represented on a log-log plot. Garrett (1989) has published capital cost-plant capacity curves for over 250 processes.

The journal *Hydrocarbon Processing* publishes supplements on refining, petrochemical, and gas processing processes every other year. These supplements are available in print or CD format to subscribers and give approximate capital cost data for various licensed processes, which can be fitted using a rearranged form of Equation 7.1:

$$C_2 = \frac{C_1}{S_1^n} \times S_2^n = a\, S_2^n \tag{7.2}$$

Values of the parameters a and n for some fuels and commodity chemical processes are given in Table 7.1. Note that these correlations are only valid over a range of plant sizes between S_{lower} and S_{upper}, corresponding to the range over which the data were fitted. The costs in the *Hydrocarbon Processing* supplements are supplied by the technology vendors and are suitable for ballpark estimates only.

TABLE 7.1 Process cost correlations

Process	Licensor	Units	Capacity			
			S_{lower}	S_{upper}	a	n
ABS resin (15% Rubber) by emulsion polymerization	Generic	MMlb/y	50	300	12.146	0.6
Acetic acid by Cativa process	BP	MMlb/y	500	2000	3.474	0.6
Acetic acid by low water methanol carbonylation	Celanese	MMlb/y	500	2000	2.772	0.6
Acrolein by propylene oxidation with Bi/Mo catalyst	Generic	MMlb/y	30	150	6.809	0.6
Adipic acid from phenol	Generic	MMlb/y	300	1000	3.533	0.6
Alkylation (sulfuric acid effluent refrigeration process)	Stratco/DuPont	bpd	4000	20,000	0.160	0.6
Alkylation (HF process)	UOP	bpd	5000	12,000	0.153	0.6
Allyl chloride by propylene chlorination	Generic	MMlb/y	80	250	7.581	0.6
Alpha olefins (full range process)	Chevron Phillips	MMlb/y	400	1200	5.240	0.6
Alpha olefins (full range process)	Shell	MMlb/y	400	1000	8.146	0.6
Benzene by sulfolane extraction	UOP/Shell	MMgal/y	50	200	7.793	0.6
Benzene by toluene hydrodealkylation	Generic	MMgal/y	50	200	7.002	0.6
Benzene reduction by Bensat process	UOP	bpd	8000	15,000	0.0275	0.6
Biodiesel (FAME) from vegetable oil	Generic	MMlb/y	100	500	2.747	0.6
bis-HET by Eastman Glycolysis	Eastman	MMlb/y	50	200	0.500	0.6
BTX Aromatics by Cyclar process	BP/UOP	tpy	200,000	800,000	0.044	0.6
BTX Aromatics by CCR Platforming process	UOP	tpy	200,000	800,000	0.015	0.6
Butadiene by extractive distillation	UOP/BASF	MMlb/y	100	500	5.514	0.6
Butadiene by Oxo-D plus extractive distillation	Texas Petrochem.	MMlb/y	100	500	11.314	0.6
Butene-1 by alphabutol ethylene dimerization	Axens	tpy	5000	30,000	0.0251	0.6
Butene-1 by BP Process	BP	tpy	20,000	80,000	0.169	0.6

Caprolactam from nitration-grade toluene	SNIA BPD S.p.A.	tpy	40,000	120,000	0.321	0.6
Carbon monoxide by steam methane reforming	Generic	MMscf/y	2000	6000	0.363	0.6
Catalytic condensation for gasoline production	UOP	bpd	10,000	30,000	0.222	0.6
Catalytic reforming by CCR platforming process	UOP	bpd	15,000	60,000	0.179	0.6
Coking by Flexicoking, including fluid coking	ExxonMobil	bpd	15,000	40,000	0.343	0.6
Coking by selective yield delayed coking	Foster Wheeler/UOP	bpd	15,000	60,000	0.109	0.68
Copolymer polypropylene by INNOVENE	BP	MMlb/y	300	900	3.430	0.6
Copolymer polypropylene by Unipol	Dow	MMlb/y	300	900	3.641	0.6
Copolymer polypropylene by SPHERIPOL Bulk	Basell	MMlb/y	300	900	3.649	0.6
Copolymer polypropylene by BORSTAR	Borealis	MMlb/y	300	900	4.015	0.6
Crude distillation by D2000	TOTAL/Technip	bpd	150,000	300,000	0.151	0.6
Cumene by Q-Max process	UOP	tpy	150,000	450,000	0.0120	0.6
Cyclic olefin copolymer by Mitsui Process	Mitsui	MMlb/y	60	120	12.243	0.6
Cyclohexane by liq-phase hydrogenation of benzene	Axens	tpy	100,000	300,000	0.0061	0.6
Dewaxing by ISODEWAXING	Chevron Lummus	bpd	6,000	15,000	0.256	0.6
2,6-Dimethylnaphthalene by MeOH alkylation	Exxon Mobil/Kobe	MMlb/y	50	100	7.712	0.6
Dimethyl terephthalate by methanolysis	Generic	MMlb/y	30	80	5.173	0.6
Dimethyl terephthalate by Huels Oxidation	Huels	MMlb/y	300	800	7.511	0.6
Ethanol by ethylene hydration	Generic	Mgal/y	30	90	9.643	0.6
Ethanol (fuel grade) by corn dry milling	Generic	tpy	100,000	300,000	0.0865	0.6
Ethylbenzene by EBOne process	ABB Lummus/UOP	tpy	300,000	700,000	0.0085	0.6

Continued

TABLE 7.1 Process cost correlations—cont'd

			Capacity			
Process	**Licensor**	**Units**	S_{lower}	S_{upper}	a	n
Ethylene by ethane cracking	Generic	MMlb/y	500	2000	9.574	0.6
Ethylene by UOP/Hydro MTO process	UOP/INEOS	MMlb/y	500	2000	8.632	0.6
Ethylene: light naphtha cracker (max ethylene)	Generic	MMlb/y	1000	2000	16.411	0.6
Ethylene by ethane/propane cracker	Generic	MMlb/y	1000	2000	7.878	0.6
Ethylene by gas oil cracker	Generic	MMlb/y	1000	2000	17.117	0.6
Ethylene glycol via ethylene oxide hydrolysis	Shell	MMlb/y	500	1000	5.792	0.6
Expandable polystyrene by suspension process	Generic	MMlb/y	50	100	3.466	0.6
Fischer Tropsch process	ExxonMobil	tpy	200,000	700,000	0.476	0.6
Fluid catalytic cracking	KBR	bpd	20,000	60,000	0.210	0.6
Fluid catalytic cracking with power recovery	UOP	bpd	20,000	60,000	0.302	0.6
Gas to liquids by Syntroleum process	Syntroleum	bpd	30,000	100,000	2.279	0.6
Gas sweetening by Amine Guard FS process	UOP	MMscf/d	300	800	0.386	0.6
Gasification by GE gasification process Maya crude	GE Energy	bpd	7000	15,000	0.681	0.6
Gasoline desulfurization, ultra-deep by Prime-G+	Axens	bpd	7000	15,000	0.0420	0.58
Glucose (40% solution) by basic wet corn milling	Generic	MMlb/y	300	800	3.317	0.6
HDPE pellets by BP gas phase process	BP Amoco	MMlb/y	300	700	3.624	0.6
HDPE pellets by Phillips slurry process	Phillips	MMlb/y	300	700	3.370	0.6
HDPE pellets by Zeigler slurry process	Zeigler	MMlb/y	300	700	4.488	0.6
High-impact polystyrene by bulk polymerization	Dow	MMlb/y	70	160	2.970	0.6
Hydrocracking by isocracking	Chevron Lummus	bpd	20,000	45,000	0.221	0.6

Hydrocracking by unicracking (distillate) process	UOP	bpd	20,000	45,000	0.136	0.66
Hydrocracking	Axens	bpd	20,000	45,000	0.198	0.6
Hydrogen by steam methane reforming	Foster Wheeler	MMscf/d	10	50	1.759	0.79
Hydrotreating by Unionfining process	UOP	bpd	10,000	40,000	0.0532	0.68
Isomerization by once-through Penex process	UOP	bpd	8,000	15,000	0.0454	0.6
Isomerization by Penex-Molex process	UOP	bpd	8000	15,000	0.120	0.6
Isophthalic acid by m-xylene oxidation	Generic	MMlb/y	160	300	9.914	0.6
Isoprene via isobutylene carbonylation	IFP	MMlb/y	60	200	10.024	0.6
Isoprene by propylene dimerization and pyrolysis	Generic	MMlb/y	60	200	6.519	0.6
Linear alkylbenzene by PACOL/DeFine/PEP/Detal[6]	UOP	MMlb/y	100	250	4.896	0.6
Linear alpha olefins	Chevron	MMlb/y	300	700	5.198	0.6
Linear alpha olefins by Linear-1 process	UOP	tpy	200,000	300,000	0.122	0.6
Maleic anhydride by fluid bed process	Generic	MMlb/y	70	150	7.957	0.6
Methacrylic acid by isobutylene oxidation	Generic	MMlb/y	70	150	7.691	0.6
Methanol via steam reforming and synthesis	Davy Process Tech.	tpd	3000	7000	2.775	0.6
m-Xylene by MX Sorbex process	UOP	MMlb/y	150	300	4.326	0.6
Naphthalene by three-stage fractional crystallizer	Generic	MMlb/y	20	50	2.375	0.6
N-Butanol from crude C4s	BASF	MMlb/y	150	300	8.236	0.6
Norbornene by Diels–Alder reaction	Generic	MMlb/y	40	90	7.482	0.6
Pentaerythritol by condensation	Generic	MMlb/y	40	90	6.220	0.6
PET resin chip with comonomer by NG3	DuPont	MMlb/y	150	300	4.755	0.6

Continued

TABLE 7.1 Process cost correlations—cont'd

Process	Licensor	Units	Capacity		a	n
			S_{lower}	S_{upper}		
Phenol from cumene (zeolite catalyst)	UOP/Sunoco	MMlb/y	200	600	6.192	0.6
Phthalic anhydride by catalytic oxidation	Generic	MMlb/y	100	200	7.203	0.6
Polycarbonate by interfacial polymerization	Generic	MMlb/y	70	150	20.680	0.6
Polyethylene terephthalate (melt phase)	Generic	MMlb/y	70	200	5.389	0.6
Polystyrene by bulk polymerization, plug flow	Generic	MMlb/y	70	200	2.551	0.6
Propylene by Oleflex process	UOP	tpy	150,000	350,000	0.0943	0.6
Propylene by metathesis	Generic	MMlb/y	500	1,000	1.899	0.6
Purified terephthalic acid	EniChem/Technimont	MMlb/y	350	700	10.599	0.6
p-Xylene by Isomar and Parex processes	UOP	tpy	300,000	700,000	0.0230	0.6
p-Xylene by Tatoray process	UOP	bpd	12,000	20,000	0.0690	0.6
Refined glycerin by distillation/adsorption	Generic	MMlb/y	30	60	2.878	0.6
Sebacic acid by cyclododecanone route	Sumitomo	MMlb/y	8	16	13.445	0.6
Sorbitol (70%) by continuous hydrogenation	Generic	MMlb/y	50	120	4.444	0.6
Styrene by SMART process	ABB Lummus/UOP	tpy	300,000	700,000	0.0355	0.6
Vinyl acetate by Cativa integrated process	BP	MMlb/y	300	800	7.597	0.6
Vinyl acetate by Celanese Vantage Process	Celanese	MMlb/y	300	800	6.647	0.6
Visbreaking by coil-type visbreaker	Foster Wheeler/UOP	bpd	6,000	15,000	0.278	0.48

Notes:
1. *Values of a are in January 2006 MM$ on a USGC basis (Nelson Farrer index = 1961.6, CEPCI index = 478.6).*
2. S_{lower} *and* S_{upper} *indicate the bounds of the region over which the correlation can be applied.*
3. S *is based on product rate for chemicals, feed rate for fuels.*
4. *If the index* n *is 0.6, then the correlation is an extrapolation around a single cost point.*
5. *Correlations are based on data taken from* Hydrocarbon Processing *(2003, 2004a,b), except where the licensor is stated as "Generic," in which case the correlations are based on data from Nexant PERP reports (see www.Nexant.com/products for a full list of reports available).*
6. *PACOL/DeFine/PEP/Detal processes.*

Economy of scale

It can be seen from the discussion earlier and the correlations in Table 7.1 that the exponent n is always less than 1.0. One result of this is that larger plants tend to cost less to construct per unit of product produced, an advantage that is known as an *economy of scale*. From Equation 7.2, the capital cost per unit of production of product will be:

$$\frac{C_2}{S_2} = a\, S_2^{n-1} \tag{7.3}$$

As $n - 1$ is less than zero, the cost per unit of production decreases as S_2 increases. A smaller capital cost per unit of product allows the owners of large plants to price their products more competitively and still recover their capital investment. This creates an incentive for chemical companies to build plants at larger scale.

7.4.2 Step count method

If cost data for a similar process are not available then an order-of-magnitude estimate can sometimes be made by adding contributions for different plant sections or functional units.

Experienced design engineers can often figure out costs of plant sections from historic total plant costs. For example, in many petrochemical processes roughly 20% of ISBL capital cost is in the reactor section and 80% is in the distillation and product purification sections. If the separation and recovery system has a similar size and complexity to that of a known process, then the capital cost can be estimated based on the cost of the known process and the reactor section cost taken as one-quarter of the separation section cost.

An alternative approach is Bridgewater's method, which correlates plant cost to the number of processing steps (Bridgewater & Mumford, 1979). For plants primarily processing liquids and solids:

$$Q \geq 60{,}000\text{: } C = 4320\, N \left(\frac{Q}{s}\right)^{0.675} \tag{7.4}$$

$$Q < 60{,}000\text{: } C = 380{,}000\, N \left(\frac{Q}{s}\right)^{0.3} \tag{7.5}$$

where: C = ISBL capital cost in US$, US Gulf Coast, January 2010 basis (CEPCI = 532.9)
Q = plant capacity in metric tons per year
s = reactor conversion (= mass of desired product per mass fed to the reactor)
N = number of functional units

(Note: The correlations have been updated from the original reference.)

A functional unit includes all the equipment and ancillaries needed for a significant process step or function, such as a reaction, separation, or other major unit operation. Pumping and heat exchange are not normally considered functional units unless they have substantial cost, for example, compressors, refrigeration systems, or process furnaces.

7.4.3 Reverse engineering methods

In some situations, a very rough estimate of capital cost can be backed out from operating costs or product prices.

Payback method

The difference between the sales price and the cost of production is the gross profit of the plant; see Section 8.2.4. If an investor were to build a new plant, then the gross profit minus taxes would have to be sufficient to give a return on the investment made in building the plant. Assuming the plant pays back in 3 to 5 years (average = 4 years), a very rough estimate of the plant cost would be:

$$\text{Plant cost} = 4 \times (\text{gross profit} - \text{taxes}) \tag{7.6}$$

For chemicals, raw materials costs are typically 80% to 90% of the cash cost of production, so the gross profit can be roughly estimated as:

$$\text{Gross profit} = \text{product value} - (1.2 \times \text{raw materials costs}) \tag{7.7}$$

This method obviously can only be used in situations where the designer believes that new plants are being built and generating a reasonable return on capital.

Turnover ratio method

An even simpler (and less accurate) method is to estimate the capital investment based on the turnover ratio. The turnover ratio is the gross annual sales divided by the fixed capital investment. The turnover ratio can vary widely, but a typical value for the chemical industry is between 1.0 and 1.25 (Humphreys, 1991).

TCOP method

For large-scale production of formed or assembled components (>500,000 pieces per year) a rule of thumb is:

$$\text{Total cost of production (TCOP)} = 2 \times \text{raw materials cost} \tag{7.8}$$

The TCOP is equal to the cost of raw materials, plus utility costs, fixed costs, and an annualized capital charge that is typically one-third to one-fifth of the capital cost (see Section 8.2.4, Equation 8.6). Equation 7.8 can thus be used to make a very approximate estimate of plant cost for manufactured products if fixed costs and utilities can be estimated.

Example 7.1

The process for making cyclohexane by saturation of benzene consists of a feed-effluent heat exchanger, a saturation reactor, and a product stabilizer column. Estimate the cost of a plant that produces 200,000 metric tons per year (200 kMTA) of cyclohexane using the correlation in Table 7.1 and Bridgewater's method.

Solution

From Table 7.1, the cost correlation for the Axens process for benzene saturation gives:

$$\begin{aligned} C &= 0.0061(S)^{0.6} \\ &= 0.0061\left(2\times 10^5\right)^{0.6} \\ &= \underline{\underline{\$9.2\ \text{MM}}} \text{ expressed on a Jan. 2006 USGC basis} \end{aligned}$$

Using Bridgewater's method, we have two functional units (the reactor and product stabilizer—the heat exchanger doesn't count), and assuming that the reactor conversion is 1.0, we can substitute into Equation 7.4:

$$\begin{aligned} C &= 4320 \times 2(Q)^{0.675} \\ &= 4320 \times 2 \times \left(2\times 10^5\right)^{0.675} \\ &= \underline{\underline{\$33\ \text{MM}}} \text{ expressed on a Jan. 2010 USGC basis} \end{aligned}$$

Note that we have obtained two very different answers. Bridgewater's correlation is known to be only an approximation; however, Table 7.1 is based on data from technology vendors that may be somewhat understated. With the level of information available, it is probably safe to say that the cost is in the range $10 MM to $20 MM. Note also that the costs are not on the same time basis. Methods for correcting costs on different time bases will be discussed in Section 7.7.

7.5 Estimating purchased equipment costs

When more design information is available, the cost of a plant can be worked up from the cost of individual items of process equipment. Costs of single pieces of equipment are also often needed for minor revamp and de-bottlenecking projects.

7.5.1 Sources of equipment cost data

The best source of purchased equipment costs is recent data on actual prices paid for similar equipment. Engineers working for engineering, procurement, and construction (EPC) companies (often referred to as *contractors*) have access to large amounts of high-quality data, as these companies carry out many projects globally every year. Engineers working in operating companies may have access to data from recent projects, but unless they work for a large company that carries out many capital projects, they are unlikely to be able to develop and maintain current cost correlations for more than a few basic equipment types. Most large companies recognize the difficulty of making reliable cost estimates and employ a few experienced cost engineering specialists who collect data and work closely with the EPC companies on project budgets.

Actual prices paid for equipment and bulk items may differ substantially from catalog or list prices, depending on the purchasing power of the contractor or client and the urgency of the project. Discounts and surcharges are highly confidential business information and will be closely guarded even within EPC companies.

Those design engineers who are outside the EPC sector and do not have the support of a cost estimating department must rely on cost data from the open literature or use cost estimating software. The most widely used software tools for estimating chemical plant costs are the Aspen Capital Cost Estimator (ACCE) suite of tools licensed by Aspen Technology, Inc., and Cleopatra Enterprise owned by Cost Engineering Consultancy. The cost estimation software within ACCE is built on the ICARUS cost estimation algorithms. ACCE does not use the factorial method, but instead estimates equipment costs, bulk costs, and installation costs from the costs of materials and labor, following the practice used by cost engineers for detailed estimating. The models in ACCE are developed by a team of cost engineers based on data collected from EPC companies and equipment manufacturers. The models are updated annually. The ACCE software is included in the standard Aspen/Hysys academic package and is available in most universities. Cleopatra Enterprise is an integrated project cost management software that supports the entire project life cycle. It uses databases of equipment costs, bulk materials costs, and installation costs that were developed from vendor quotations and historic data and are updated annually. Cleopatra's database allows cost estimates to be built in different levels of detail, supporting the preparation of high-level, semi-detailed, and detailed estimates that cover the full scope of a project. The software also has a variety of features for analyzing and comparing different estimates and scenarios. Both ACCE and Cleopatra can give reasonably good estimates when used properly, and both are described in more detail in Section 7.10.

There is an abundance of equipment cost data and cost correlations in the open literature, but much of it is of very poor quality. The relationship between size and cost given in Equations 7.1 and 7.2 can also be used for equipment if a suitable size parameter is used. If the size range spans several orders of magnitude, then log-log plots usually give a better representation of the relationship than simple equations.

Some of the most reliable information on equipment costs can be found in the professional cost engineering literature. Correlations based on recent data are occasionally published in *Cost Engineering*, which is the journal of AACE International. AACE International also has an excellent website, www.aacei.org, which has cost models that can be used by members. There is also an extensive listing of other web resources for cost estimating at https://web.aacei.org/resources/publications. The UK Association of Cost Engineers (ACostE) publishes the journal *The Cost Engineer* and also prints a guide to capital cost estimating (Gerrard, 2000), which gives cost curves for the main types of process equipment based on recent data. The prices are given in British pounds sterling on a UK basis, but this book is useful for making estimates of prices in northwest Europe. The International Cost Engineering Council website (www.icoste.org) provides links to 46 international cost engineering societies, several of which maintain databases of local costs.

Current prices for new and used equipment can be found on resale websites such as www.equipnet.com. It is not always easy to find the exact piece of equipment needed on such sites, but they can be used to give a good indication of the accuracy of cost correlations. A free web-based costing tool is available at www.matche.com. This tool appears to have not been updated since 2003, and the source of the cost correlations given is not clear, so it is not suitable for any use other than undergraduate design projects.

Many cost correlations can be found in chemical engineering textbooks, for example, Douglas (1988), Garrett (1989), Turton et al. (2003), Peters et al. (2003), Ulrich and Vasudevan (2004), and Seider et al. 2016). The references for such correlations should always be checked very carefully. When they are properly referenced, they are often found to be based on data published by Guthrie (1969, 1974) and updated using either cost indices (as described in Section 7.7) or a few recent data points. Guthrie's correlations were reasonably good when published, but there have been substantial changes in the relative contributions of material and fabrication costs of most process equipment since then. Academic authors usually do not have access to sufficient high-quality cost data to be able to make

reliable correlations, and most of the academic correlations predict lower costs than would be obtained using ACCE or other detailed estimating methods. These correlations are adequate for the purposes of university design projects but should not be used in real projects. It is to be hoped that the authors of these publications will benchmark their correlations against ACCE or Cleopatra in future editions, which will improve the accuracy of the correlations and make them more useful to those who do not have access to costing software.

7.5.2 Cost curves for purchased equipment costs

For those design engineers who lack access to reliable cost data or estimating software, the correlations given in Table 7.2 can be used for preliminary estimates. The correlations in Table 7.2 are of the form:

$$C_e = a + b\,S^n \tag{7.9}$$

where: C_e = purchased equipment cost on a U.S. Gulf Coast basis, Jan. 2010 (CEPCI = 532.9, NF refinery inflation index = 2281.6)
a, b = cost constants in Table 7.2
S = size parameter, units given in Table 7.2
n = exponent for that type of equipment

The correlations in Table 7.2 are only valid between the lower and upper values of S indicated. The prices are all for carbon steel equipment except where noted in the table. Extrapolation to other materials is discussed in Section 7.6.3.

Example 7.2

Estimate the purchased equipment cost of a plain carbon steel shell and tube heat exchanger with area 400 m^2.

Solution

From Table 7.2, the cost correlation for a shell and tube heat exchanger is:

$$C_e = 28,000 + 54\,A^{1.2} \tag{7.9}$$

where A is the area in m^2 and C_e is on a January 2010 basis. Substituting for the area:

$$C_e = 28,000 + \left(54 \times 400^{1.2}\right) = \underline{\underline{\$99,600}}$$

7.5.3 Detailed method of cost estimating

When the method of design and construction of a piece of equipment are known, the cost can be estimated from the costs of the materials, parts, labor, and manufacturer's profit. This is the method preferred by professional cost estimators and procurement managers, as it allows the estimator to obtain an unbiased estimate of the real cost of the equipment, which can then be used in negotiations with the vendor to determine a fair price. This method is also used in many of the correlations in commercial cost estimating programs such as ACCE.

A detailed estimate requires an itemized list of the required parts, an understanding of the fabrication steps, knowledge of the machinery involved (so as to estimate the machine costs), and an understanding of the amount of labor needed for each step. The fabrication method is stated as a work breakdown structure (WBS) to arrive at an accurate estimate of the labor. Machine time costs are usually allocated by taking the annual cost of the machine, including allowances for capital recovery, maintenance, and electric power costs, and then dividing these costs by the number of hours in use to arrive at an hourly machine cost. The overall cost can then be made by summing the component costs, machine costs, and labor costs and adding suitable amounts for supervision, overhead, and manufacturer's profit. A hypothetical example of a cost breakdown structure for a shell and tube heat exchanger is given in Table 7.3.

The detailed method of cost estimating must be followed whenever cost or price data are not available, for example, when making an estimate of the cost of specialized equipment that cannot be found in the literature. For example, a reactor design is usually unique for a particular process but the design can be broken down into

TABLE 7.2 Purchased equipment cost for common plant equipment

Equipment	Units for size, S	S_{lower}	S_{upper}	a	b	n	Note
Agitators and mixers							
Propeller	driver power, kW	5.0	75	17,000	1130	1.05	
Spiral ribbon mixer	driver power, kW	5.0	35	30,800	125	2.0	
Static mixer	liters/s	1.0	50	570	1170	0.4	
Boilers							
Packaged, 15 to 40 bar	kg/h steam	5000	200,000	124,000	10.0	1.0	
Field erected, 10 to 70 bar	kg/h steam	20,000	800,000	130,000	53	0.9	
Centrifuges							
High-speed disk	diameter, m	0.26	0.49	57,000	480,000	0.7	
Atmospheric suspended basket	power, kW	2.0	20	65,000	750	1.5	
Compressors							
Blower	m^3/h	200	5000	4450	57	0.8	
Centrifugal	driver power, kW	75	30,000	580,000	20,000	0.6	
Reciprocating	driver power, kW	93	16,800	260,000	2700	0.75	
Conveyors							
Belt, 0.5 m wide	length, m	10	500	41,000	730	1.0	
Belt, 1.0 m wide	length, m	10	500	46,000	1320	1.0	
Bucket elevator, 0.5 m bucket	height, m	10	30	17,000	2600	1.0	
Crushers							
Reversible hammer mill	t/h	30	400	68,400	730	1.0	
Pulverizers	kg/h	200	4000	16,000	670	0.5	
Jaw crusher	t/h	100	600	−8000	62,000	0.5	
Gyratory crusher	t/h	200	3000	5000	5100	0.7	
Ball mill	t/h	0.7	60	−23,000	242,000	0.4	
Crystallizers							
Scraped surface crystallizer	length, m	7	280	10,000	13,200	0.8	
Distillation columns							
See pressure vessels, packing, and trays							
Dryers							
Direct contact rotary	area, m^2	11	180	15,000	10,500	0.9	1
Atmospheric tray batch	area, m^2	3.0	20	10,000	7900	0.5	
Spray dryer	evap rate kg/h	400	4,000	410,000	2200	0.7	
Evaporators							
Vertical tube	area, m^2	11	640	330	36,000	0.55	
Agitated Falling film	area, m^2	0.5	12	88,000	65,500	0.75	2

Continued

TABLE 7.2 Purchased equipment cost for common plant equipment—cont'd

Equipment	Units for size, S	S_{lower}	S_{upper}	a	b	n	Note
Exchangers							
U-tube shell and tube	area, m^2	10	1000	28,000	54	1.2	
Floating head shell and tube	area, m^2	10	1000	32,000	70	1.2	
Double pipe	area, m^2	1.0	80	1900	2500	1.0	
Thermosiphon reboiler	area, m^2	10	500	30,400	122	1.1	
U-tube Kettle reboiler	area, m^2	10	500	29,000	400	0.9	
Plate and frame	area, m^2	1.0	500	1600	210	0.95	2
Filters							
Plate and frame	capacity, m^3	0.4	1.4	128,000	89,000	0.5	
Vacuum drum	area, m^2	10	180	−73,000	93,000	0.3	
Furnaces							
Cylindrical	duty, MW	0.2	60	80,000	109,000	0.8	
Box	duty, MW	30	120	43,000	111,000	0.8	
Packings							
304 ss Raschig rings	m^3			0	8000	1.0	
Ceramic Intalox saddles	m^3			0	2000	1.0	
304 ss pall rings	m^3			0	8500	1.0	
PVC structured packing	m^3			0	5500	1.0	
304 ss structured packing	m^3			0	7600	1.0	3
Pressure vessels							
Vertical, cs	shell mass, kg	160	250,000	11,600	34	0.85	4
Horizontal, cs	shell mass, kg	160	50,000	10,200	31	0.85	4
Vertical, 304 ss	shell mass, kg	120	250,000	17,400	79	0.85	4
Horizontal, 304 ss	shell mass, kg	120	50,000	12,800	73	0.85	4
Pumps and drivers							
Single-stage centrifugal	flow liters/s	0.2	126	8000	240	0.9	
Explosion proof motor	power, kW	1.0	2500	−1100	2100	0.6	
Condensing steam turbine	power, kW	100	20,000	−14,000	1900	0.75	
Reactors							
Jacketed, agitated	volume, m^3	0.5	100	61,500	32,500	0.8	2
Jacketed, agitated, glass lined	volume, m^3	0.5	25	12,800	88,200	0.4	
Tanks							
Floating roof	capacity, m^3	100	10,000	113,000	3250	0.65	
Cone roof	capacity, m^3	10	4000	5800	1600	0.7	
Trays							
Sieve trays	diameter, m	0.5	5.0	130	440	1.8	5
Valve trays	diameter, m	0.5	5.0	210	400	1.9	
Bubble cap trays	diameter, m	0.5	5.0	340	640	1.9	

TABLE 7.2 Purchased equipment cost for common plant equipment—cont'd

Equipment	Units for size, S	S_{lower}	S_{upper}	a	b	n	Note
Utilities							
Cooling tower and pumps	flow liters/s	100	10,000	170,000	1500	0.9	6
Packaged mechanical refrigerator	evaporator duty, kW	50	1,500	24,000	3500	0.9	
Water ion exchange plant	flow m^3/h	1	50	14,000	6200	0.75	

Notes:
1. Direct heated.
2. Type 304 stainless steel.
3. With surface area 350 m^2/m^3.
4. Not including heads, ports, brackets, internals, etc. (see Chapter 14 for how to calculate wall thickness).
5. Cost per tray, based on a stack of 30 trays.
6. Field assembly.
7. All costs are U.S. Gulf Coast basis, Jan. 2010 (CEPCI index = 532.9, NF refinery inflation index = 2281.6).

TABLE 7.3 Hypothetical cost breakdown for fabrication of a heat exchanger

Step	Materials	Parts	Machine	Labor
1. Shell fabrication				
1.1 Shell forming	Steel plate, $L_s \times \pi D_s \times t_s$		Cutting Rolling Welding	2 hr 2 hr 2 hr
1.2 End flange forming	Two steel plate discs, D_f diameter $\times$ t_f		Cutting Drilling (for bolt holes)	1 hr each 2 hr each
1.3 Flange attachment			Welding	2 hr each
1.4 Nozzle reinforcement	Two steel plate discs, 2 D_n diameter		Cutting/rolling Welding	2 hr 1 hr each
1.5 Nozzle attachment		Two flanged pipes	Welding	1 hr each
2. Head fabrication (×2) (Note: Both nozzles may be on one head, depending on the exchanger type.)				
2.1 Head forming	Steel plate disc		Cutting Drop forging	1 hr
2.2 Hole cutting			Cutting	4 hr
2.3 End flange forming	Two steel plate discs, D_f diameter $\times$ t_f		Cutting Drilling (for bolt holes)	1 hr 2 hr
2.4 Flange attachment			Welding	2 hr
2.5 Nozzle reinforcement	Two steel plate discs, D_n diameter		Cutting/rolling Welding	1 hr each 1 hr each
2.6 Nozzle attachment		Two flanged pipes	Welding	1 hr each
3. Tube bundle fabrication				
3.1 Tube sheet fabrication	Steel plate disc, D_s diameter		Stamping	1 hr
3.2 Baffle cutting	N_{baf} steel plate discs		Stamping	0.5 hr each
3.3 Tie rod cutting	10 to 12 $\times$ L, steel rod		Cutting Threading	1 hr 2 hr
3.4 Tube preparation	N_t tubes cut to right length		Cutting Bending	0.25 hr each 0.25 hr each

Continued

TABLE 7.3 Hypothetical cost breakdown for fabrication of a heat exchanger—cont'd

Step	Materials	Parts	Machine	Labor
3.5 Bundle assembly				0.25 hr/tube
3.6 Tube sheet sealing			Welding/rolling	0.25 hr/tube
4. Exchanger assembly				
4.1 Bundle insertion			Large crane	1hr
4.2 Gasket cutting	Two sheets gasket material		Stamping	1 hr
4.3 Head attachment		N_b bolts		2 hr

Notes:
1. L_s = *shell length*, D_s = *shell diameter*, t_s = *shell thickness*, D_f = *flange diameter*, t_f = *flange thickness*, D_n = *nozzle diameter*, N_{baf} = *number of baffles*, N_t = *number of tubes*, N_b = *number of bolts*.
2. *Dimensions are not exact, labor hours are approximate, and some steps have been omitted to simplify the example. There could be considerable variation in labor times depending on the exchanger layout and complexity.*
3. *Costs would also include supervision, testing and inspection, overhead, and manufacturer's margin.*
4. *The components and fabrication of a shell and tube heat exchanger are discussed in detail in Chapter 19.*

standard components (vessels, heat-exchange surfaces, spargers, agitators, etc.), the cost of which can be found in the literature and used to build up an estimate of the reactor cost.

More information on estimating costs from a detailed breakdown of parts and labor is given by Dysert (2015) in the AACE International's training manual (Hastak, 2015). Breakdowns of the materials and labor components for many types of process equipment are given by Page (1996). Pikulik and Diaz (1977) give a method of costing major equipment items from cost data on the basic components: shells, heads, nozzles, and internal fittings. Purohit (1983) gives a detailed procedure for estimating the cost of heat exchangers.

7.5.4 Use of vendor data in cost estimating

At some point in the development of a design it is always necessary to get a real price quotation from an equipment vendor. Although vendor quotations are always realistic, some caution is needed to ensure that such estimates are valid for the use intended.

A large amount of vendor information is now available online and can easily be found using any of the major search engines or by starting from directories such as www.purchasing.com. Online costs are usually manufacturer's catalog prices for small-order quantities. Large order sizes (as filled by contractors) are often heavily discounted, which is one reason why many operators subcontract plant construction to EPC companies that have greater purchasing power. Items requiring special fabrication, for example, large vessels or compressors, may experience discounts or surcharges depending on the state of the manufacturer's order books and the purchasing power of the customer.

When a vendor is contacted directly, the quality of estimate that they can provide depends very much on the quality of the information that they are given. Often the vendor will ask the customer to provide information on the process conditions and equipment duty, so as to be able to complete their own optimization and ensure that the model or design specified is correct for the purpose. It is very important to include any constraints on materials of construction in the specification provided to the vendor, as materials substitution can cause significant increases in cost; see Section 7.6.3.

As with any purchasing decision, it is always a good idea to contact several vendors and comparison shop for the best price. Care must be taken to be ethical in handling vendors' confidential information, and commercially sensitive information such as pricing should not be shared with other vendors.

7.6 Estimating installed costs: The factorial method

Capital cost estimates for chemical process plants are often based on an estimate of the purchase cost of the major equipment items required for the process, with the other costs being estimated as factors of the equipment cost. The accuracy of this type of estimate will depend on what stage the design has reached at the time the estimate is made

TABLE 7.4 Installation factors proposed by Hand (1958)

Equipment type	Installation factor
Compressors	2.5
Distillation columns	4
Fired heaters	2
Heat exchangers	3.5
Instruments	4
Miscellaneous equipment	2.5
Pressure vessels	4
Pumps	4

and on the reliability of the data available on equipment costs. In the later stages of the project design, when detailed equipment specifications are available and firm quotes have been obtained from vendors, a Class 3 estimate of the capital cost of the project can be made by this method, but generally this method leads to a Class 4 estimate.

7.6.1 Lang factors

Lang (1948) proposed that the ISBL fixed capital cost of a plant is given as a function of the total purchased equipment cost by the equation:

$$C = F\left(\sum C_e\right) \tag{7.10}$$

where: C = total plant ISBL capital cost (including engineering costs).
ΣC_e = total delivered cost of all the major equipment items: reactors, tanks, columns, heat exchangers, furnaces, etc. The delivered cost is the purchased cost plus shipping or delivery costs.
F = an installation factor, later widely known as a *Lang factor.*

Lang originally proposed the following values of F, based on 1940s economics:

$F = 3.1$ for solids processing plants
$F = 4.74$ for fluids processing plants
$F = 3.63$ for mixed fluids-solids processing plants

Hand (1958) suggested that better results are obtained by using different factors for different types of equipment. Examples of the factors proposed by Hand are given in Table 7.4. Hand also observed that this approach should only be used in the earliest stages of process design and in the absence of detailed design information.

Both Lang (1948) and Hand (1958) included home office costs but not offsite costs or contingency in their installation factors, so beware of double counting EPC costs when using this approach. The relative costs of materials and labor have changed substantially from when these factors were developed, and the accuracy of the correlation probably never warranted three significant figures for F. Most practitioners using this method therefore use a Lang factor of 3, 4, or 5, depending on the plant scale (larger plant = smaller factor) and type.

7.6.2 Detailed factorial estimates

Equation 7.10 can be used to make a preliminary estimate once the flowsheet has been drawn up and the main plant equipment has been sized. When more detailed design information is available, the installation factor can be estimated somewhat more rigorously by considering the cost factors that are compounded into the Lang factor individually.

The direct-cost items that are incurred in the construction of a plant in addition to the delivered cost of equipment are:

1. Equipment erection, including foundations and minor structural work
2. Piping, including insulation and painting
3. Electrical, power, and lighting
4. Instruments and automatic process control (APC) systems
5. Process buildings and structures
6. Ancillary buildings, offices, laboratory buildings, and workshops (if not costed separately as offsites)
7. Storage for raw materials and finished product (if not costed separately as offsites)
8. Utilities and provision of plant for steam, water, air, and firefighting services (if not costed separately as offsites)
9. Site preparation

The contribution of each of these items to the total capital cost is calculated by multiplying the total purchased equipment cost by an appropriate factor. As with the basic Lang factor, these factors are best derived from historical cost data for similar processes. Typical values for the factors are given in several references: Happle and Jordan (1975) and Garrett (1989). Guthrie (1974) splits the costs into the material and labor portions and gives separate factors for each.

The accuracy and reliability of an estimate can be further improved by dividing the process into subunits and using factors that depend on the function of the subunits; see Guthrie (1969). In Guthrie's detailed method of cost estimation, the installation, piping, and instrumentation costs for each piece of equipment are costed separately. Detailed costing is only justified if the cost data available are reliable and the design has been taken to the point where all the cost items can be identified and included. Gerrard (2000) gives factors for individual pieces of equipment as a function of equipment cost and complexity of installation.

Typical factors for the components of the capital cost are given in Table 7.5. These can be used to make an approximate estimate of capital cost using equipment cost data published in the literature.

7.6.3 Materials factors

The installation factors given in Tables 7.4 and 7.5 are for plants built from carbon steel. When more exotic materials are used, a materials factor f_m should also be introduced:

TABLE 7.5 Typical factors for estimation of project fixed capital cost

	Process type		
Item	**Fluids**	**Fluids–solids**	**Solids**
1. Major equipment, total purchase cost	C_e	C_e	C_e
f_{er} Equipment erection	0.3	0.5	0.6
f_p Piping	0.8	0.6	0.2
f_i Instrumentation and control	0.3	0.3	0.2
f_{el} Electrical	0.2	0.2	0.15
f_c Civil	0.3	0.3	0.2
f_s Structures and buildings	0.2	0.2	0.1
f_l Lagging and paint	0.1	0.1	0.05
ISBL cost, $C = \Sigma C_e \times$	3.3	3.2	2.5
Offsites (OS)	0.3	0.4	0.4
Design and Engineering (D&E)	0.3	0.25	0.2
Contingency (X)	0.1	0.1	0.1
Total fixed capital cost $C_{FC} = C$ (1 + OS)(1 + D&E + X)			
$= C \times$	1.82	1.89	1.82
$= \Sigma C_e \times$	6.00	6.05	4.55

$$f_m = \frac{\text{purchased cost of item in exotic material}}{\text{purchased cost of item in carbon steel}} \tag{7.11}$$

Note that f_m is not equal to the ratio of the metal prices, as the equipment purchased cost also includes labor costs, overheads, fabricator's profit, and other costs that do not scale directly with metal price. Equation 7.10 can then be expanded for each piece of equipment to give:

$$C = \sum_{i=1}^{i=M} C_{e,i,CS}\,[(1+f_p)f_m + (f_{er}+f_{el}+f_i+f_c+f_s+f_l)] \tag{7.12}$$

Equation 7.12 should be used when the purchased equipment cost has been found on a carbon steel basis and the designer is estimating the cost for alloy construction. If the purchased equipment cost has been obtained on an alloy basis, then the designer should instead correct the other installation factors so as not to overestimate the cost of installation:

$$C = \sum_{i=1}^{i=M} C_{e,i,A}\,[(1+f_p) + (f_{er}+f_{el}+f_i+f_c+f_s+f_l)/f_m] \tag{7.13}$$

where: $C_{e,i,CS}$ = purchased equipment cost of equipment i in carbon steel
$C_{e,i,A}$ = purchased equipment cost of equipment i in alloy
M = total number of pieces of equipment
f_p = installation factor for piping
f_{er} = installation factor for equipment erection
f_{el} = installation factor for electrical work
f_i = installation factor for instrumentation and process control
f_c = installation factor for civil engineering work
f_s = installation factor for structures and buildings
f_l = installation factor for lagging, insulation, or paint

Failure to properly correct installation factors for materials of construction is one of the most common sources of error with the factorial method. Typical values of the materials factor for common engineering alloys are given in Table 7.6. A more detailed discussion of the relative cost of materials and sources of material cost factors is given in Section 6.6.

7.6.4 Summary of the factorial method

Many variations of the factorial method are used. The method outlined here can be used with the data given in this chapter to make a quick, approximate estimate of the fixed capital investment needed for a project.

TABLE 7.6 Materials cost factors, f_m, relative to plain carbon steel

Material	f_m
Carbon steel	1.0
Aluminum and bronze	1.07
Cast steel	1.1
304 stainless steel	1.3
316 stainless steel	1.3
321 stainless steel	1.5
Hastelloy C	1.55
Monel	1.65
Nickel and Inconel	1.7

1. Prepare material and energy balances; draw up preliminary flowsheets; size major equipment items and select materials of construction.
2. Estimate the purchased cost of the major equipment items; see Section 7.5.
3. Calculate the ISBL installed capital cost, using the factors given in Table 7.5 and correcting for materials of construction using Equation 7.12 or 7.13 with the materials factors given in Table 7.6.
4. Calculate the OSBL, engineering, and contingency costs using the factors given in Table 7.5.
5. The sum of ISBL, OSBL, engineering, and contingency costs is the fixed capital investment.
6. Estimate the working capital as a percentage of the fixed capital investment; 10% to 20% is typical (or, better, calculate it from the cost of production if this has been estimated—see Section 9.2.3).
7. Add the fixed and working capital to get the total investment required.

Example 7.3

A plant modification has been proposed that will allow recovery of a by-product. The modification consists of adding the following equipment:

Distillation column, height 30 m, diameter 3 m, 50 sieve trays, operating pressure 10 bar

- U-tube heat exchanger, area 60 m^2
- Kettle reboiler, area 110 m^2
- Horizontal pressure vessel, volume 3 m^3, operating pressure 10 bar
- Storage tank, volume 50 m^3
- Two centrifugal pumps, flow rate 3.6 m^3/h, driver power 500 W
- Three centrifugal pumps, flow rate 2.5 m^3/h, driver power 1 kW (two installed plus one spare)

Estimate the installed ISBL capital cost of the modification if the plant is to be built from type 304 stainless steel. Estimate the cost using both Hand's method and the factors given in Table 7.5.

Solution

The first step is to convert the units to those required for the correlations and determine any missing design information. The distillation column can be costed as a combination of a vertical pressure vessel and internals. For both pressure vessels we need to know the wall thickness. The details of how to calculate vessel wall thickness in accordance with the ASME Boiler and Pressure Vessel Code are given in Section 14.5, and the equation to use is Equation 14.13.

The design pressure of the vessels should be 10% above the operating pressure (see Chapter 14), so the design pressure is 11 bar, or roughly 1.1×10^6 N/m^2. The maximum allowable stress for type 304 stainless steel at 500 °F (260 °C) is 12.9 ksi or roughly 89 N/mm^2 (see Table 14.2). Assuming the welds will be fully radiographed, the weld efficiency is 1.0. Substituting in Equation 14.13 for the column wall thickness, t_w, then gives:

$$t_w = \frac{1.1 \times 10^6 \times 3}{(2 \times 89 \times 10^6 \times 1.0) - (1.2 \times 1.1 \times 10^6)} \quad (14.13)$$
$$= 0.0187 \text{ m, say } 20 \text{ mm}$$

We can now calculate the shell mass, using the density of 304 stainless steel (= 8000 kg/m^3, from Table 6.2).

$$\text{Shell mass} = \pi D_c L_c t_w \rho$$

where: D_c = vessel diameter, m
L_c = vessel length, m
t_w = wall thickness, m
ρ = metal density, kg/m^3

So the shell mass for the distillation column is:

$$\text{Shell mass} = \pi \times 3.0 \times 30 \times 0.02 \times 8000 = 46685 \text{ kg}$$

For the horizontal pressure vessel we need to convert the volume into a length and diameter. Assuming that the vessel is a cylinder with $L_c = 2D_c$ then we can follow the same method as for the column and find $t_w = 8$ mm and shell mass = 636 kg.

Using the correlations in Table 7.2, we obtain the following purchased costs for the stainless steel pressure vessels:

$$\text{Distillation column shell, cost} = 17,400 + 79\ (46685)^{0.85} = \$753,000$$

$$\text{Horizontal pressure vessel, cost} = 12,800 + 73\ (636)^{0.85} = \$30,400$$

For the remaining equipment we obtain the following purchased costs from the correlations in Table 7.2 based on carbon steel construction:

Distillation column trays, cost per tray $= 130 + 440\,(3.0)^{1.8}$	$= \$3310$
Cost for 50 trays	$= \$165{,}500$
U − tube heat exchanger, cost $= 28{,}000 + 54\,(60)^{1.2}$	$= \$35{,}300$
Kettle reboiler, cost $= 29{,}000 + 400\,(110)^{0.9}$	$= \$56{,}500$
Storage tank (conical head), cost $= 5800 + 1600(50)^{0.7}$	$= \$30{,}500$
Centrifugal pump, $3.6\ m^3/h = 1L/s$, SO:	
cost each $= 8000 + 240(1.0)^{0.9} = \$8240$, cost for two pumps	$= \$16{,}480$
driver (electric motor) cost each $= -1100 + 2{,}100(0.5)^{0.6}$	$= \$285$
cost for two drivers	$= \$570$
Centrifugal pump, $2.5\ m^3/h = 0.694\ L/s$, so	
cost each $= 8000 + 240\,(0.694)\,0.9 = \$8170$, cost for three	$= \$24{,}520$
driver (electric motor) cost each $= -1100 + 2100(1.0)^{0.6}$	$= \$1000$
cost for three drivers	$= \$3000$

Note that the pumps and drivers are at the lower end of the range of validity of the cost correlations and the driver cost for the smaller motors looks suspect; however, the pump and motor costs are small compared with the other costs, and the error introduced is therefore negligible given the overall accuracy of ±30%.

Following Hand's method, the installed cost of the distillation column is then:

$$C = 4 \times 753{,}000 = \$3{,}012{,}000$$

The cost of the trays can be converted to type 304 stainless steel by multiplying by the appropriate materials factor from Table 7.6, giving:

$$C = 1.3 \times 165{,}500 = \$215{,}150$$

This then gives a total cost for the column plus internals of 3,012,000 + 215,150 = $3,227,150.

The installed cost of the horizontal pressure vessel is 4 × 30,400 = $121,600.

The installed cost for the exchangers and storage tank in carbon steel construction is:

$$C = 3.5(35{,}300 + 56{,}500) + 2.5(30{,}500) = \$397{,}550$$

so the cost in type 304 stainless steel is 1.3 × 397,550 = $516,800.

For the pumps, we need to add the cost of the pump and driver before determining the installed cost. Only the cost of the pump needs to be converted to stainless steel. For the first set of pumps:

$$C = 4 \times (570 + (1.3 \times 16{,}480)) = \$88{,}000$$

For the second set of pumps only two are installed (the other is a warehouse spare), so the total installed cost is:

$$C = (1.3 \times 8170) + 1000 + (4 \times 2 \times (1000 + (1.3 \times 8170))) = \$105{,}000$$

The total installed ISBL cost of the plant is then:

$$C = 3{,}227{,}150 + 121{,}600 + 516{,}800 + 88{,}000 + 105{,}000 = \$4{,}058{,}550$$

or $\underline{\$4.1\ MM \pm 30\%}$ within the accuracy of the method.

If instead we use the factors given in Table 7.5, then using Equation 7.12, the installed cost for the exchangers, tank, and pumps is equal to:

$$C = (35{,}300 + 56{,}500 + 30{,}500 + 16{,}480 + 8170)[(1 + 0.8) \times 1.3 + (0.3 + 0.3 + 0.2 + 0.3 + 0.2 + 0.1)]$$

$$C = (155{,}120)[3.74] = \$580{,}150$$

The installed cost for the pump drivers (which do not require a materials conversion factor) is:

$$C = (1140 + 6{,}000)[1 + 0.8 + 0.3 + 0.3 + 0.2 + 0.3 + 0.2 + 0.1]$$
$$C = (7140)[3.2] = \$22{,}900$$

The installed cost for the pressure vessels can be found using Equation 7.13:

$$C = (753{,}000 + 30{,}400)[1 + 0.8 + (0.3 + 0.3 + 0.2 + 0.3 + 0.2 + 0.1)/1.3]$$
$$C = (783{,}400)[2.88] = \$2{,}256{,}200$$

In addition to this, we require the cost of the trays in stainless steel and the cost of the spare pump and driver:

$$C = 1000 + 1.3(165{,}500 + 8170) = \$226{,}800$$

The total installed ISBL cost of the plant is then:

$$C = 580{,}150 + 22{,}900 + 2{,}256{,}200 + 226{,}800 = \$3{,}086{,}050$$

or $\underline{\$3.1\ \text{MM} \pm 30\%}$ within the accuracy of the method.

Note that although the answers obtained by the two methods are different, the second answer is within the range of accuracy of the first, and the first is very close to the upper end of the range predicted by the second method. Both estimates should be stated as being on a U.S. Gulf Coast basis, January 2010, as this is the basis for the correlations in Table 7.2.

7.7 Cost escalation

All cost estimating methods use historical data and are themselves forecasts of future costs. The prices of the materials of construction and the costs of labor are subject to inflation. Some method has to be used to update old cost data for use in estimating at the design stage and to forecast the future construction cost of the plant.

The method usually used to update historical cost data makes use of published cost indices. These relate present costs to past costs and are based on data for labor, material, and energy costs published in government statistical digests.

$$\text{Cost in year A} = \text{Cost in year B} \times \frac{\text{Cost index in year A}}{\text{Cost index in year B}} \tag{7.14}$$

To get the best estimate, each job should be broken down into its components, and separate indices should be used for labor and materials. It is often more convenient to use the composite indices published for various industries in the trade journals. These are weighted average indices combining the various components of costs in proportions considered typical for the particular industry.

A composite index for the U.S. process plant industry is published monthly in the journal *Chemical Engineering*; this is the Chemical Engineering Plant Cost Index (CEPCI), often referred to as the *CE index*. *Chemical Engineering* also used to publish the Marshall and Swift index (M&S equipment cost index), but that index has been discontinued since 2010.

For oil refinery and petrochemicals projects, the *Oil and Gas Journal* used to publish the Nelson-Farrar Refinery Construction Index (NF index). The index is now available as a subscription service from https://www.bakerrisk.com/products/nelson-farrar-cost-index/. The index is updated monthly, and indices for 40 types of equipment are updated quarterly. The Nelson-Farrar index is on a U.S. Gulf Coast basis rather than U.S. average, and is more reliable than the CE index for the types of equipment used in hydrocarbon processing.

The journal *Engineering News Record* publishes a monthly construction cost index. This is based on civil engineering projects and is sometimes used for updating offsite costs. This index has been published since 1904 and is the oldest of all the indices.

For international projects, the journal *Process Engineering* publishes monthly cost indices for several countries, including the United States, United Kingdom, Japan, Australia, and many of the EU countries.

All cost indices should be used with caution and judgment. They do not necessarily relate the true make-up of costs for any particular piece of equipment or plant, nor the effect of supply and demand on prices. The longer

the period over which the correlation is made, the more unreliable the estimate. Between 1970 and 1990 prices rose dramatically. Prices then grew at a more or less steady 2% to 3% per year until 2003, when high demand for fuels projects and high energy prices caused another period of steeper price inflation. Prices then decreased during the 2008–2010 recession before another period of growth driven by major projects associated with the U.S. shale gas expansion and downstream petrochemical investments. At time of writing, the indices have not yet shown any impact of the 2020 COVID-19 pandemic and resulting economic recession and oil price crash; however, it is likely that there will be a substantial decrease in the indices in 2020 and that recovery to 2019 levels will not occur until there is renewed capital investment in the fuels and chemicals sector. The major cost indices are plotted in Fig. 7.2. Fig. 7.3 shows the same data plotted relative to the 1990 value of each index. Fig. 7.3 shows that the NF index is usually a leading indicator compared with the M&S and CE indices, as fuels-sector activity has been a big component of price inflation from 2000 onwards.

To estimate the future cost of a plant, some prediction has to be made of the future annual rate of cost inflation. This can be based on the extrapolation of one of the published indices, tempered by the engineer's own assessment of what the future may hold. Inflation is difficult to forecast, and allowance for inflation is often included in the contingency charges added to the project cost.

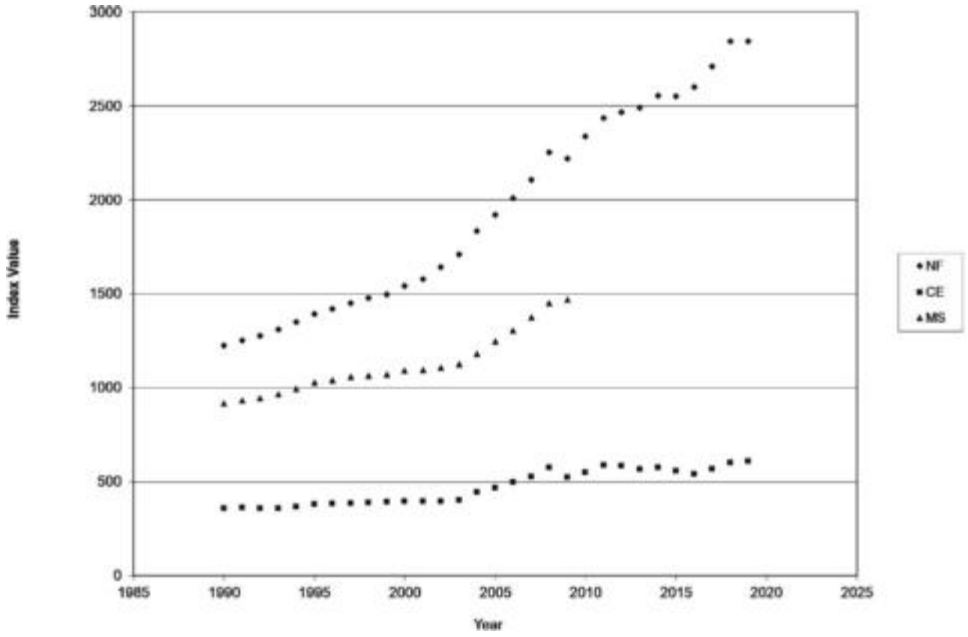


FIG. 7.2 Variation of major cost indices.

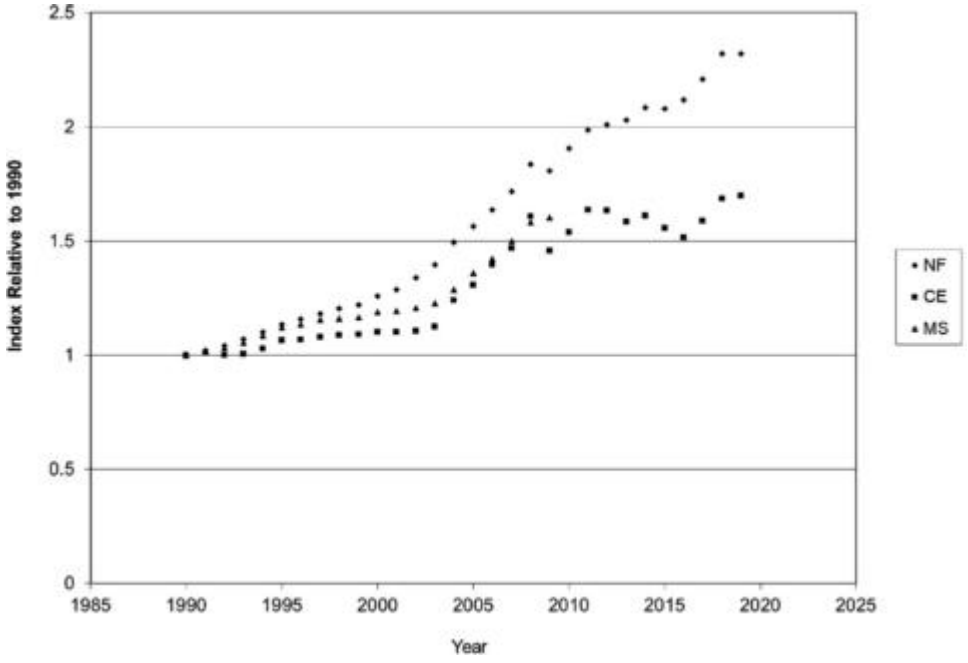


FIG. 7.3 Variation of major cost indices relative to 1990 = 1.0.

Example 7.4

The purchased cost of a shell and tube heat exchanger, carbon shell, 316 stainless steel tubes, heat transfer area 500 m^2, was \$64,000 in January 2003; estimate the cost in January 2020. Use the CEPCI Equipment Cost Index.

Solution

From Fig. 7.2 (or by looking up the index in *Chemical Engineering*):

Index in 2003 = 402

Index in January 2020 = 596

So, estimated cost in January 2020 = \$64,000 × 596 / 402 = \$95,000

Example 7.5

The purchased cost of a distillation column was \$136,000 in 2004. Estimate the cost in 2024. Use the Nelson-Farrer index.

Solution

From Fig. 7.2 (or by looking up the index in *Oil and Gas Journal*):

Index in 2004 = 1833.6

The index in 2024 is difficult to extrapolate numerically, as it is not yet clear how deep or long the 2020 recession will be, nor whether we will see another sharp increase afterwards, as experienced in 2015–2018. Looking at Fig. 7.2, it seems likely that the NF index will have a value in the range of 3000 to 3200. A conservative approach would be to make a higher estimate, so let us assume 3200.

So, estimated cost in January 2022 = \$136,000 × 3200 / 1833.6 = \$237,000

7.8 Location factors

Most plant and equipment cost data are given on a U.S. Gulf Coast (USGC) or northwest Europe (NWE) basis, as these were historically the main centers of the chemical industry, for which the most data were available. The cost of building a plant in any other location will depend on:

- Local fabrication and construction infrastructure
- Local labor availability and cost
- Costs of shipping or transporting equipment to site
- Import duties or other local tariffs
- Currency exchange rates, which affect the relative cost of locally purchased items such as bulk materials, when converted to a conventional pricing basis such as U.S. dollars

These differences are captured in cost estimating by using a location factor:

$$\text{Cost of plant in location A} = \text{cost of plant on USGC} \times LF_A \tag{7.15}$$

where: LF_A = location factor for location A relative to USGC basis

Location factors for international locations are a strong function of currency exchange rates and hence fluctuate with time. Cran (1976a,b), Bridgewater (1979), Soloman (1990), and Gerrard (2000) give location factors for international locations from which this variation can be seen. It can be argued that as a result of globalization, all international installation factors are trending closer to 1.0 (Gerrard, 2000). Location factors within a country are somewhat

TABLE 7.7 Location factors

Country	Region	Location factor
United States	Gulf Coast	1.00
	East Coast	1.04
	West Coast	1.07
	Midwest	1.02
Canada	Ontario	1.00
	Fort McMurray	1.60
Mexico		1.03
Brazil		1.14
China	imported	1.12
	indigenous	0.61
Japan		1.26
Southeast Asia		1.12
Australia		1.21
India		1.02
Middle East		1.07
France		1.13
Germany		1.11
Italy		1.14
Netherlands		1.19
Russia		1.53
United Kingdom		1.02

easier to predict, and Bridgewater (1979) suggested a simple rule of thumb: add 10% for every 1000 miles from the nearest major industrial center.

Table 7.7 gives example location factors. These are based on data from Aspen Richardson's *International Construction Cost Factor Location Manual* (2003). More recent versions of this manual can be found by searching for Richardson Engineering Services at www.aspentech.com. The values in Table 7.7 give costs on a local basis in U.S. dollars. The location factors in Table 7.7 are based on 2003 data and can be updated by dividing by the ratio U.S. dollar/local currency in 2003 and multiplying by the ratio U.S. dollar/local currency in the year of interest. If a cost estimate for a future year is being made, then currency variation will have to be forecasted.

Example 7.6

The cost of constructing a 30,000 metric tons per year (30 kMTA) acrolein plant was estimated as $80 million ($80MM) on a 2006 U.S. Gulf Coast basis. What would be the cost in U.S. dollars on a 2006 Germany basis?

Solution

From Table 7.7, the 2003 location factor for Germany was 1.11.

The exchange rate in 2003 averaged about €1 = $1.15, and in 2006 it averaged about €1 = $1.35.

The 2006 location factor for Germany is thus $1.11 \times 1.35/1.15 = 1.30$

The cost of building the acrolein plant in Germany in 2006 is $80 MM $\times$ 1.30 = $\underline{\underline{\$104\ MM}}$

7.9 Estimating off-site capital costs

Improvements to the site infrastructure are almost always needed when a new plant is added to a site or a major expansion is carried out. The cost of such improvements is known as the *off-site or OSBL investment*, as described in Section 7.2.1.

In the early stages of designing a new process, the off-site requirements are usually not precisely known, and an allowance for off-site costs can be made by assuming that they will be a ratio of the ISBL investment. A typical number is 30% to 50% of ISBL investment, depending on the process and site conditions. Table 7.8 gives some guidelines for making approximate estimates of off-site capital costs as a function of plant complexity and site conditions.

TABLE 7.8 Guidelines for estimating approximate OSBL costs as a percentage of ISBL cost

	Site condition		
Process complexity	**Existing: underused**	**Existing: tight capacity**	**New site**
Typical large-volume chemical	30%	40%	40%
Low-volume specialty chemical	20%	40%	50%
High solids-handling requirement	40%	50%	100%

As the design details are established and the requirements for utilities such as steam, electricity, and cooling water are determined, the site requirements can also be determined. If there is insufficient spare capacity in the existing site infrastructure, potential modifications can be designed to accommodate the new plant. For existing sites, the design engineer must always beware of scope creep, in which the new project is used to justify all kinds of (possibly long overdue) improvements to the site infrastructure. If scope creep occurs, excessive off-site costs may make the project economics unattractive.

Many of the off-site items are designed as "packaged" plants or systems that are purchased from specialized suppliers. In some cases, the supplier may even offer an *over-the fence* contract, in which the supplier builds, owns, and operates the off-site plant and contracts to supply the site with the desired utility stream or service. Over-the-fence contracts are widely used for industrial gases such as nitrogen, oxygen, and hydrogen, and most plants also import electricity from the local utility company. Over-the-fence contracts for steam, cooling water, and effluent treatment are less common, but are sometimes used in smaller plants or where several companies share a site.

The question of whether to build a self-contained infrastructure for a plant or contract for off-site services is an example of a *make-or-buy* problem. The over-the-fence price will usually be higher than the cost of producing the utility or service internally, because the supplier needs to make a profit and recover their capital investment. On the other hand, contracting for the service reduces the project capital investment and fixed costs, because the supplier must take on the costs of labor, maintenance, and overheads. The make-or-buy decision is usually made by comparing annualized costs, as described in Section 9.7.2. Correlations for costs of utility plants and other off-sites are given in the sources listed in Section 7.5.

7.10 Computer tools for cost estimating

It is difficult for engineers outside the EPC sector to collect recent cost data from a large set of real projects and maintain accurate and up-to-date cost correlations. Instead, the most common method for making preliminary estimates in industry is to use commercial cost estimating software.

A wide variety of cost estimating programs is available. These include ACCE (Aspen Technology, Inc.), Cleopatra Enterprise (Cost Engineering Consultancy), CostLink/CM (Building Systems Design, Inc.), Cost Track (OnTrack Engineering Ltd.), PRISM Project Estimator (ARES Corp.), Success Estimator (U.S. Cost), Visual Estimator (CPR International Inc.), WinEst (Win Estimator), and others that can be found by searching on the Web or looking at the listings provided by AACE International at www.aacei.org. The discussion in this section will focus on the most widely used programs: Aspen Technology's ACCE software and Cost Engineering Consultancy's Cleopatra Enterprise. Both of these programs have academic licenses available for university use and are also available in most chemical companies.

The ACCE and Cleopatra cost estimating tools are simple to use and give quick, defensible estimates without requiring a lot of design data. Design information can be uploaded from major flowsheet simulation programs or entered manually. The programs allow the design to be updated as more information on design details becomes available, so that a more accurate estimate can be developed. Costs can be estimated for a whole plant or for one piece of equipment at a time. Both programs include a large number of equipment types, and these can be designed in a broad range of materials, including U.S., UK, German, and Japanese standard alloys.

Both ACCE and Cleopatra use a combination of mathematical models and expert systems to develop cost estimates. Costs are based on the materials and labor required (following the practice used for detailed estimates) rather than installation factors. If design parameters are not specified by the user, then they are calculated or set to default values by the program. The user should always review the design details carefully to make sure that the default values make sense for the application. If any values are not acceptable, they can be manually adjusted and a more realistic estimate can be generated.

A detailed description of how to run ACCE or Cleopatra is beyond the scope of this book. Both programs have user manuals available from the licensor or as .pdf files downloadable from the "help" button in the program, see, for example, AspenTech (2002a,b). Some of the common issues that arise in using these programs are discussed next. These or similar problems are also faced when using other cost estimating software.

7.10.1 Mapping simulation data

Instructions on loading data from a process simulation are given in the ACCE User's Guide (AspenTech, 2002a). When a simulator report file is loaded, ACCE generates a block-flow diagram with each unit operation of the simulation shown as a block. These blocks must then be "mapped" to ICARUS project components (pieces of equipment or bulk items).

Unless the user specifies otherwise, each simulator block is mapped to a default ICARUS project component. The mapping defaults need to be understood properly, as large errors can be introduced if unit operations are mapped incorrectly. The default mapping specifications are given in section 3 of the user's guide (AspenTech, 2002a). Some mappings that commonly cause problems include:

1. Reactors: Plug-flow reactor models (PLUG in Hysys and ProII, RPLUG in AspenPlus) are mapped to a packed tower, which is fine for fixed-bed catalytic reactors, but not for other types of plug-flow reactors. All other reactor models (Gibbs, stoichiometric, equilibrium, and yield) are mapped to agitated tank reactors. Reactors that are not suitable for these mappings can be mapped to other ICARUS project components or set up as user models (see later).
2. Heaters, coolers, and heat exchangers: The default mapping for all heat transfer equipment is the floating head heat exchanger. ICARUS contains several different heat exchanger types, including a generic TEMA heat exchanger that can be customized to the other types, as well as fired heater and air cooler components. It is often worthwhile to change the default mapping to the TEMA exchanger to allow the exchangers to be customized in ICARUS.
3. Distillation columns: The simulator column models include not just the column itself but also the reboiler, condenser, overhead receiver drum, and reflux pump (but not bottoms pump). ICARUS has 10 possible configurations to which a column can be mapped. Alternatively, the column can be mapped to a packed or trayed tower, and the ancillary items can be created as separate ICARUS project components.
4. Dummy items: Process simulations often contain models of items that are not actual plant equipment (see Chapter 4). For example, heat exchangers are sometimes modeled as a series of heaters and coolers linked by a calculator block as a means of checking for internal pinch points or allowing for heat losses to the ambient environment. When the simulation is mapped into ICARUS, dummy items should be excluded from the mapping process. In the previous example, only the heaters should be mapped, so as to avoid double counting the heat transfer area.

The default mapping can be edited by right-clicking on "Project Component Map Specifications" in the Project Basis/Process Design folder. A simulator model can be excluded from the mapping by selecting the item and then selecting "Delete All Mappings." New mappings can be specified by selecting a simulator item and adding a new mapping.

To map loaded simulator data, click the map button on the toolbar (which maps all items) or right-click on an area or plant item in the process view window (which allows items to be mapped individually). If individual items are selected, then the user is given an option to use simulator data to override the default mapping in the Component

Map Specs file. This is useful for heat exchangers and other equipment where the simulator allows the equipment type to be specified.

The procedure for mapping equipment in Cleopatra is somewhat simpler and is illustrated in Example 7.7.

7.10.2 Design factors in ACCE

All good designs include an appropriate degree of overdesign to allow for uncertainties in the design data and method; see Section 1.6. For some equipment, the design factor or margin is specified by design codes and standards, for example, in the design of pressure vessels, as described in Chapter 14. In other cases, the design engineer must specify the degree of overdesign or margin based on experience, judgment, or company policy.

The equipment sizes calculated by a process simulator will be at the design flow rate unless a higher throughput was specified by the user, and hence include no design margin. The ACCE software adds an "equipment design allowance" to the equipment cost to allow for the design factor that will be introduced when the equipment is designed in detail. The equipment design allowance is based on the process description as follows:

New and unproven process	15%
New process	10%
Redesigned process	7%
Licensed process	5%
Proven process	3%

The process description is entered by right-clicking on "General Specs" in the Project Basis/Basis for Capital Costs folder.

The equipment design allowance is only applied to system-developed costs. If different design margins are needed for different equipment types, then the default should be set to "proven process," and the equipment can then be oversized appropriately. Design margins can also be added to components using the ACCE custom model tool. Care should be taken to avoid adding more design margin than is necessary.

7.10.3 Pressure vessels

When costing pressure vessels such as reactors and distillation columns, care must be taken to ensure that the wall thickness is adequate. The default method in both ACCE and Cleopatra calculates the wall thickness required based on the ASME Boiler and Pressure Vessel Code Section VIII Division 1 method for the case where the wall thickness is governed by containment of internal pressure (see Chapter 14 for details of this method). If other loads govern the design, then the ACCE software can significantly underestimate the vessel cost. This is particularly important for vessels that operate at pressures below 5 bara, where the required wall thickness is likely to be influenced by dead weight loads and bending moments from the vessel supports, and for tall vessels such as distillation columns and large packed-bed reactors, where combined loading under wind loads may govern the thickness. Similarly, if the vessel is designed under a different section of the Boiler and Pressure Vessel Code, which is usually the case for vessels operated at high pressures, then ACCE can overestimate the vessel cost. It is important to always remember to enter the design pressure and temperature of the vessel, not the operating pressure and temperature.

The best approach to costing pressure vessels using commercial costing software is to enter all of the dimensions after completing the mechanical design of the vessel using the methods given in Chapter 14, or using suitable pressure vessel design software.

7.10.4 Nonstandard components in ACCE

Although ACCE contains over 250 equipment types, many processes require equipment that is not on the list of available project components. Also, in some cases the user will want to specify a certain make or model of equipment that may only be available in discrete sizes (for example, gas turbine engines or large pumps and compressors). In these situations, the nonstandard equipment can be included by setting up an Equipment Model Library (EML). Many companies maintain standard EMLs listing equipment that they often specify.

A new EML can be created by selecting the "Libraries" tab in the palette and opening the folder Cost Libraries/Equipment Model Library. Right-clicking on either of the subfolders then allows the user to create a new EML in the appropriate set of units. Once an EML has been created, equipment items can be added to it. When a new item is added, a dialog box opens in which the user has to specify the sizing or costing method (linear, log-log, semi-log or discrete) and primary sizing parameters. Two costs and sizes must also be entered to establish the cost correlation.

Equipment model libraries are useful for completing an ACCE model of a process that contains nonstandard items. Care must be taken to update the EML costs so that they remain current.

Example 7.7

Estimate the cost of a waste heat boiler designed to produce 4000 lb/h of steam. The exchanger area has been estimated as 1300 ft^2.

Solution in ACCE

Starting from the ACCE project explorer window (on the far left of the screen), right-click on the Main Area and select Add Project Component (Fig. 7.4a).

Select Process Equipment, then Heat Exchangers (Fig. 7.4b). Select Waste Heat Boiler and enter a name (Fig. 7.4c).

Enter the size parameters and then click the Evaluate button (Fig. 7.4d). This runs the evaluator program and gives the results screen shown in Fig. 7.4e. The purchased equipment cost is $145,900 on a Jan. 2006 USGC basis. The installed cost is $196,225. Note that the installed cost is calculated directly by estimating bulk materials and labor rather than using an installation factor.

Solution in Cleopatra Enterprise

Starting from the Database Explorer (top-right menu), create a new document for the estimate (Fig. 7.4f, label A). Select the Estimating tab and then select the Equipment Knowledgebase tab, and in the Level tab select Unit-rates (Fig. 7.4f, label B). Then work through the drop-down menus to select Process Equipment / Special packaged mechanical equipment / Boilers / Steam boiler / Water tube packaged boiler (Fig. 7.4f, label C).

Clicking on the waste heat boiler then opens the menu for that item (Fig. 7.4g) and allows the user to add it to the shopping cart (label A) and open the data entry window by clicking the pyramid plus icon (label B). The equipment data can then be entered (Fig. 7.4h). The flow rate of 4000 lb/h corresponds to a duty of roughly 1220 kW, and we can select 40 bar as the operating pressure (a reasonable value for high-pressure steam). Cleopatra Enterprise then returns an equipment cost of $119,000 on a Jan. 2018 U.S. basis, and we can add this into an overall estimate by clicking the pyramid button at the bottom right to give the results page shown in Fig. 7.4i.

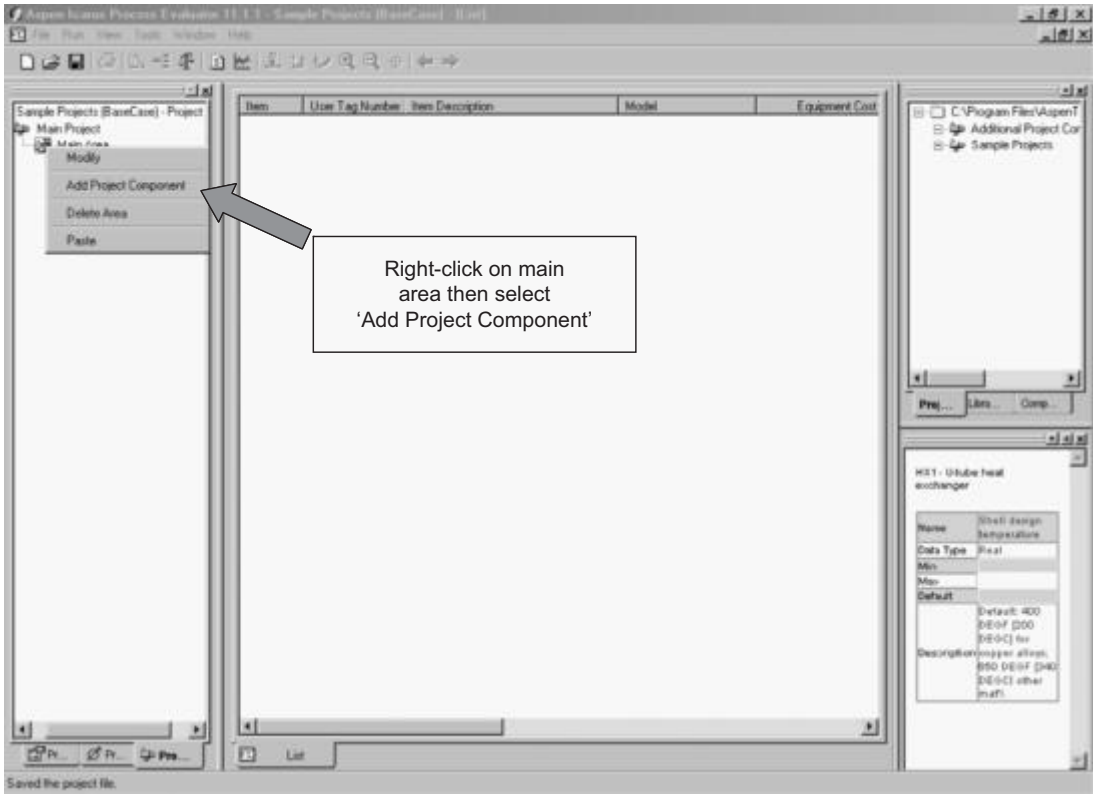
The cost generated by Cleopatra Enterprise is a bare-module cost for the equipment. We would need to enter more details about the plant layout and associated instrumentation and piping to generate an installed cost (or use a suitable Hand factor).

Note that the two programs do not give identical answers. This is a common occurrence when using costing software, as the different programs are based on different data sets. An experienced cost engineer will benchmark the results from the software against recent cost data for equipment they have purchased and tune the costing models to more accurately fit their experience of local costs. Tuning of the cost models is beyond the scope of this book, but is typically covered in the software user manuals.

7.11 Validity of cost estimates

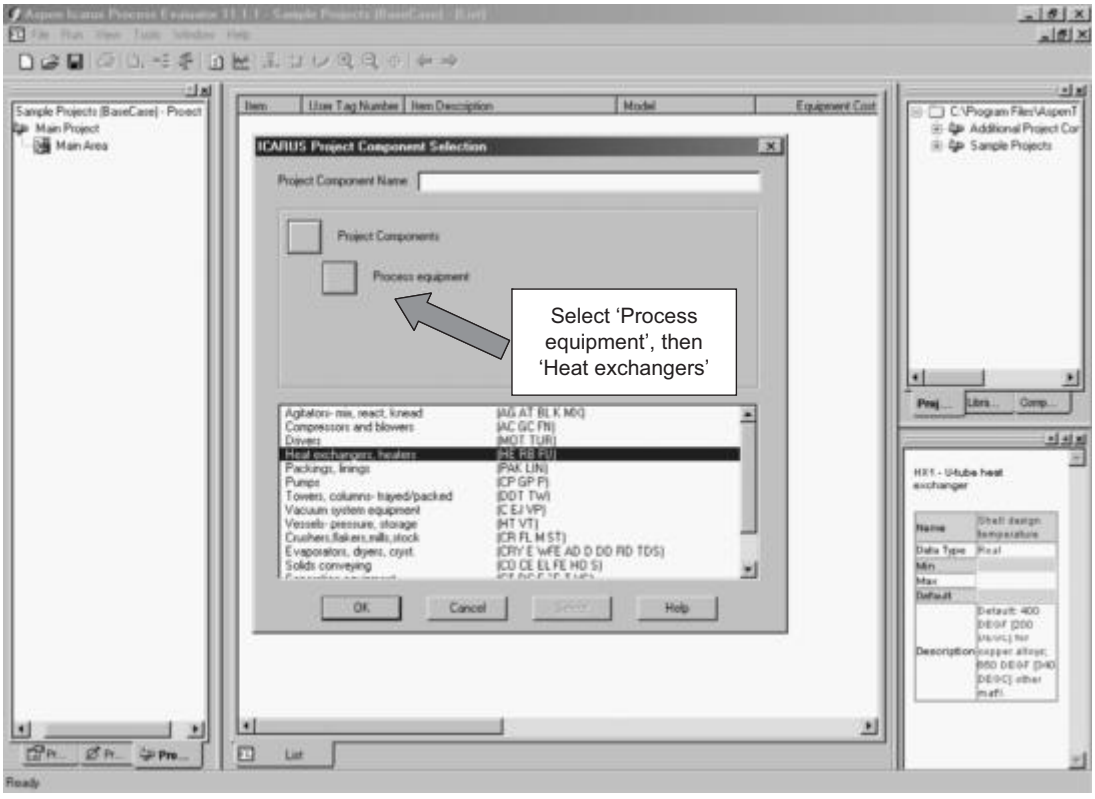
It should always be remembered that cost estimates are only estimates and are subject to error. An estimate should always indicate the margin of error. The error in a cost estimate is primarily determined by the degree of design detail that is available, and even a skilled estimator cannot estimate an accurate cost for an incomplete design.

When more design information has been developed, a professional cost engineer will be able to develop a more accurate estimate. The process design engineer should compare this estimate with the preliminary estimate to gain a better understanding of where the preliminary estimate could have been improved (either through capturing missing plant items or using better costing methods). This will help the design engineer to produce better preliminary estimates in the future.



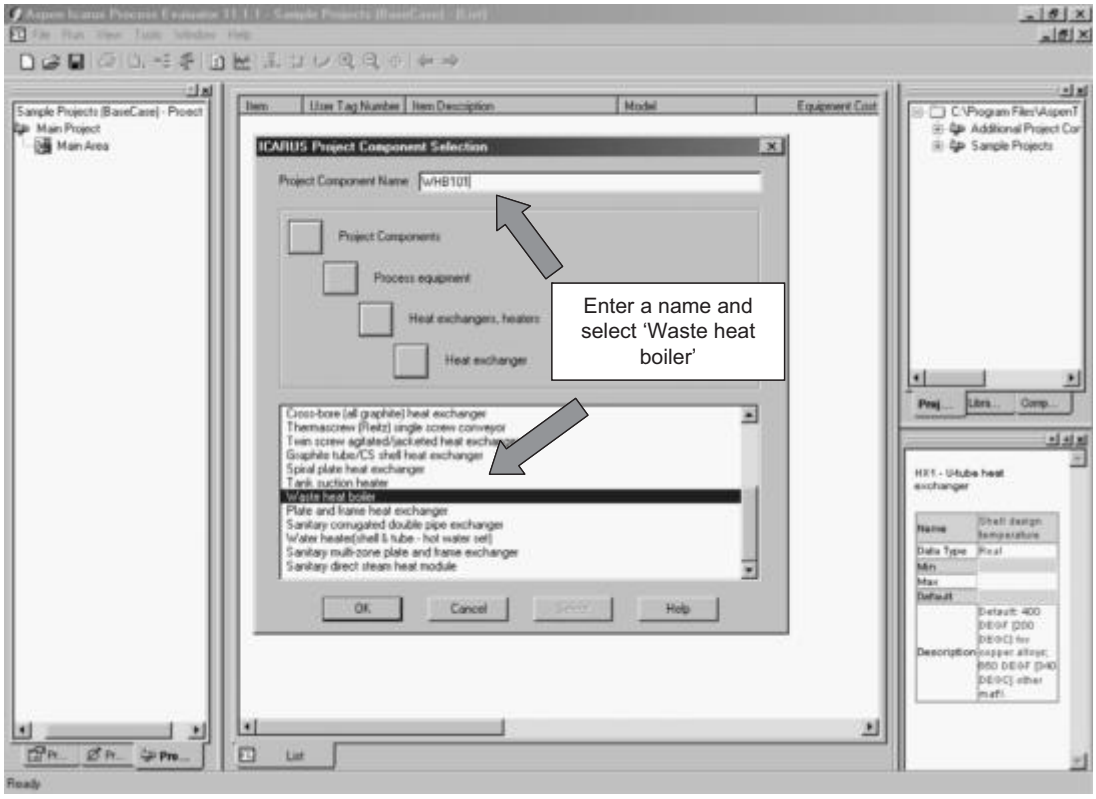
(a)

FIG. 7.4 (a–e) ACCE example. (f–i) Cleopatra Enterprise example.



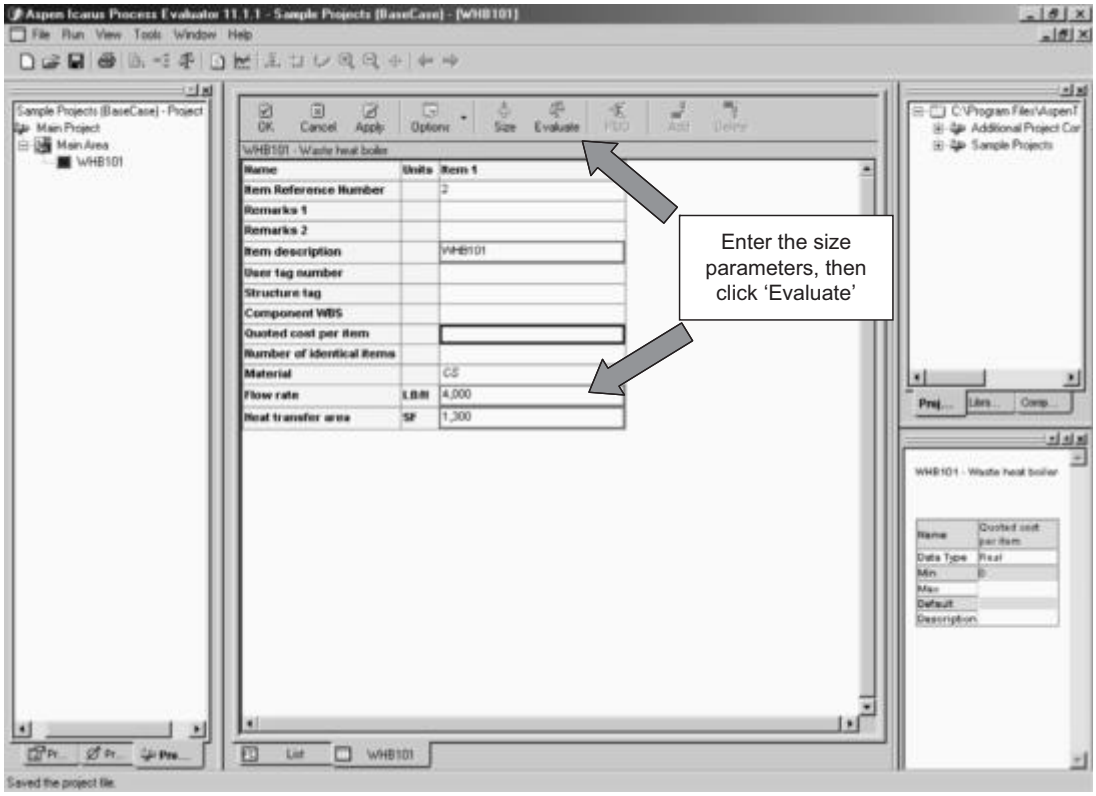
(b)

FIG. 7.4 Cont'd.



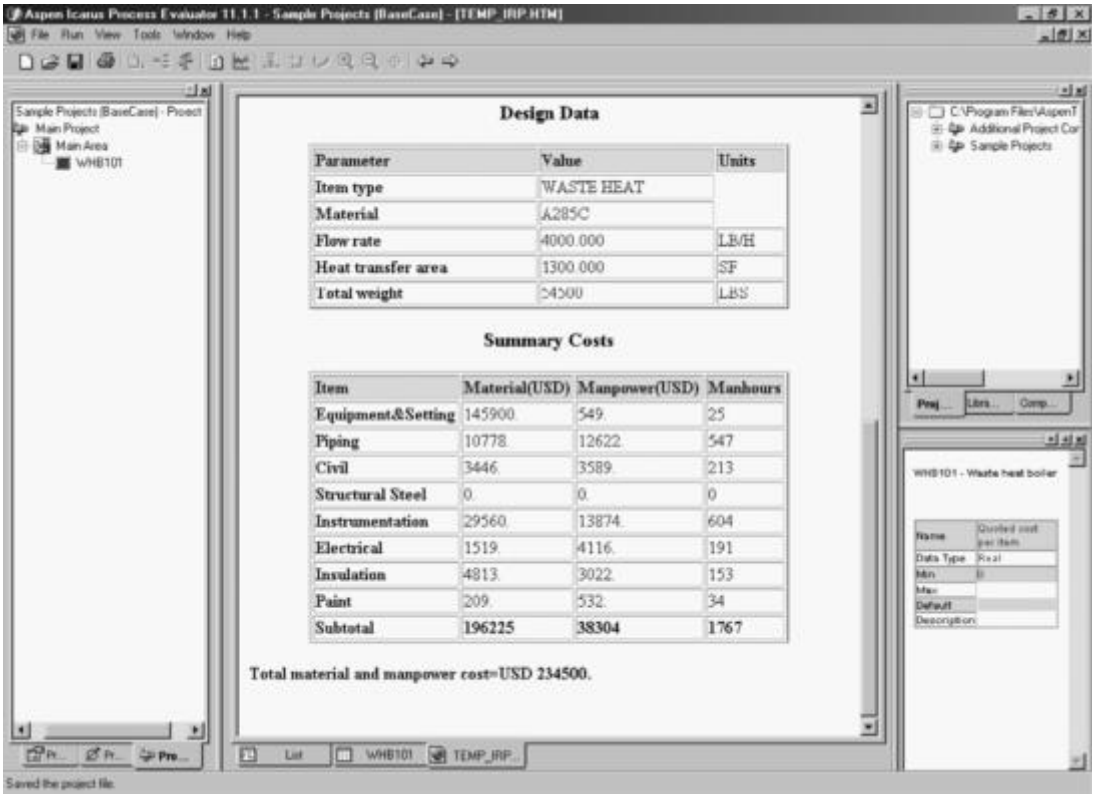
(c)

FIG. 7.4 Cont'd.



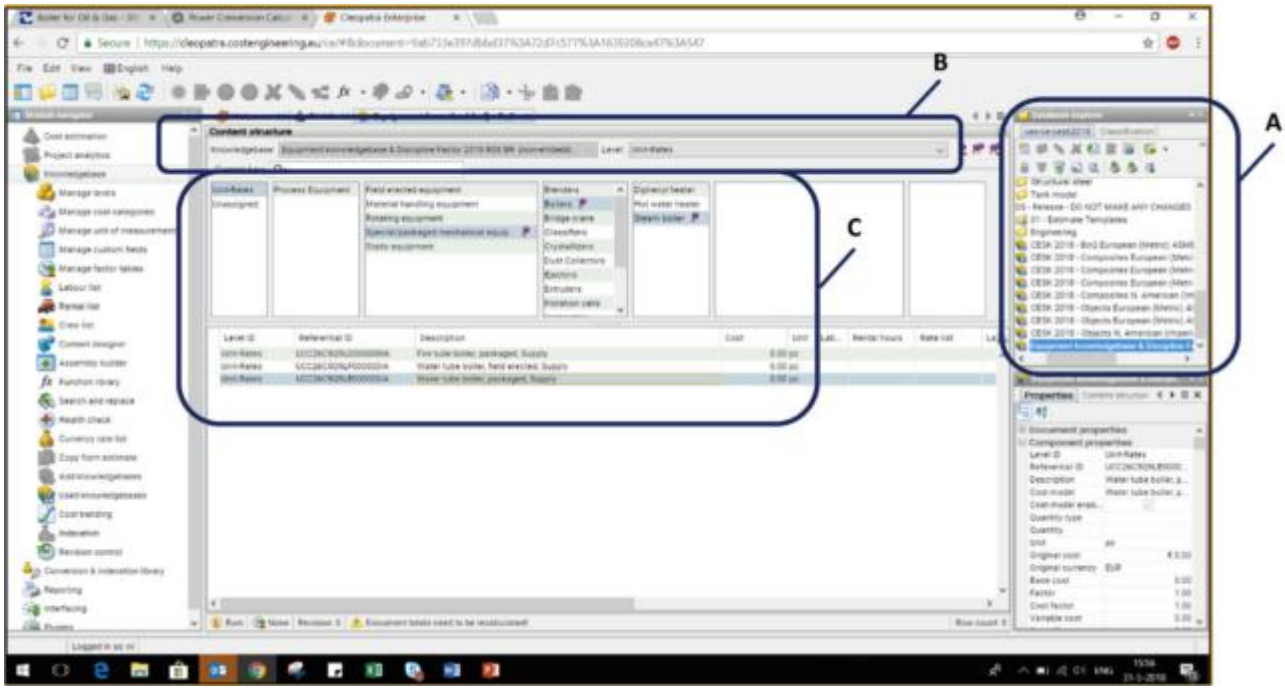
(d)

FIG. 7.4 Cont'd.



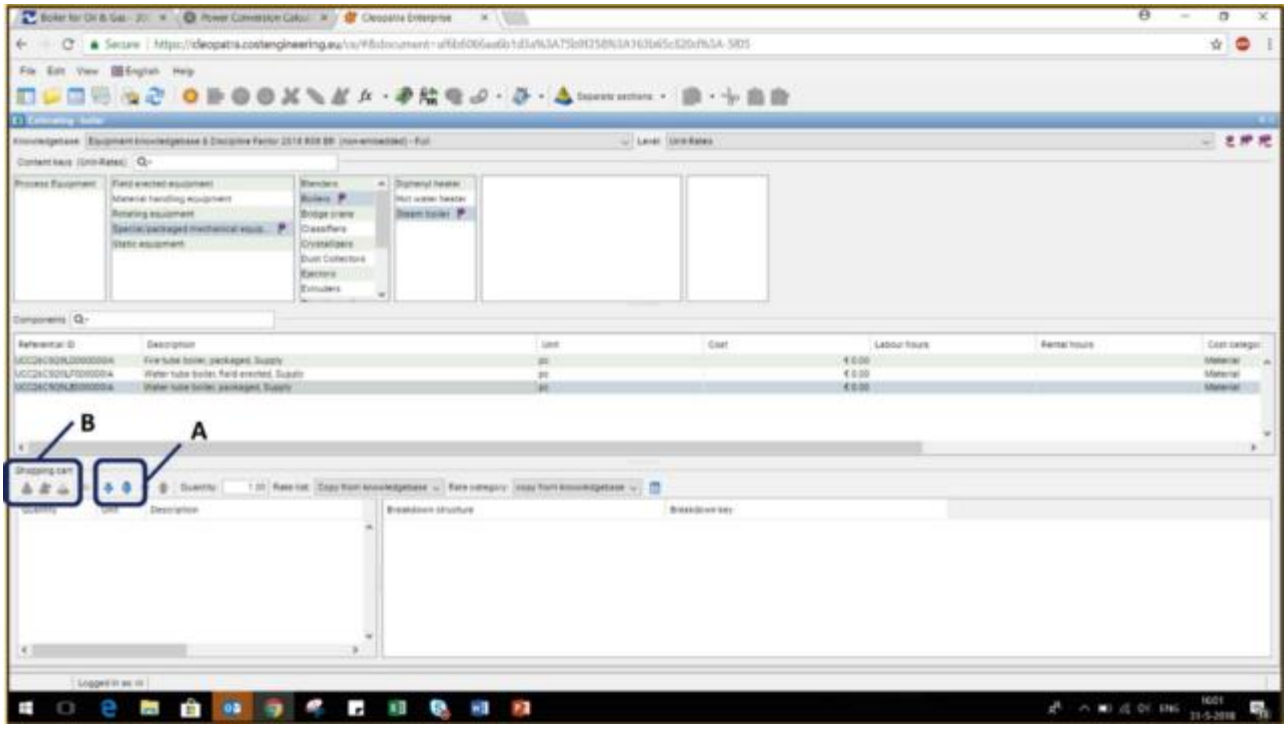
(e)

FIG. 7.4 Cont'd.



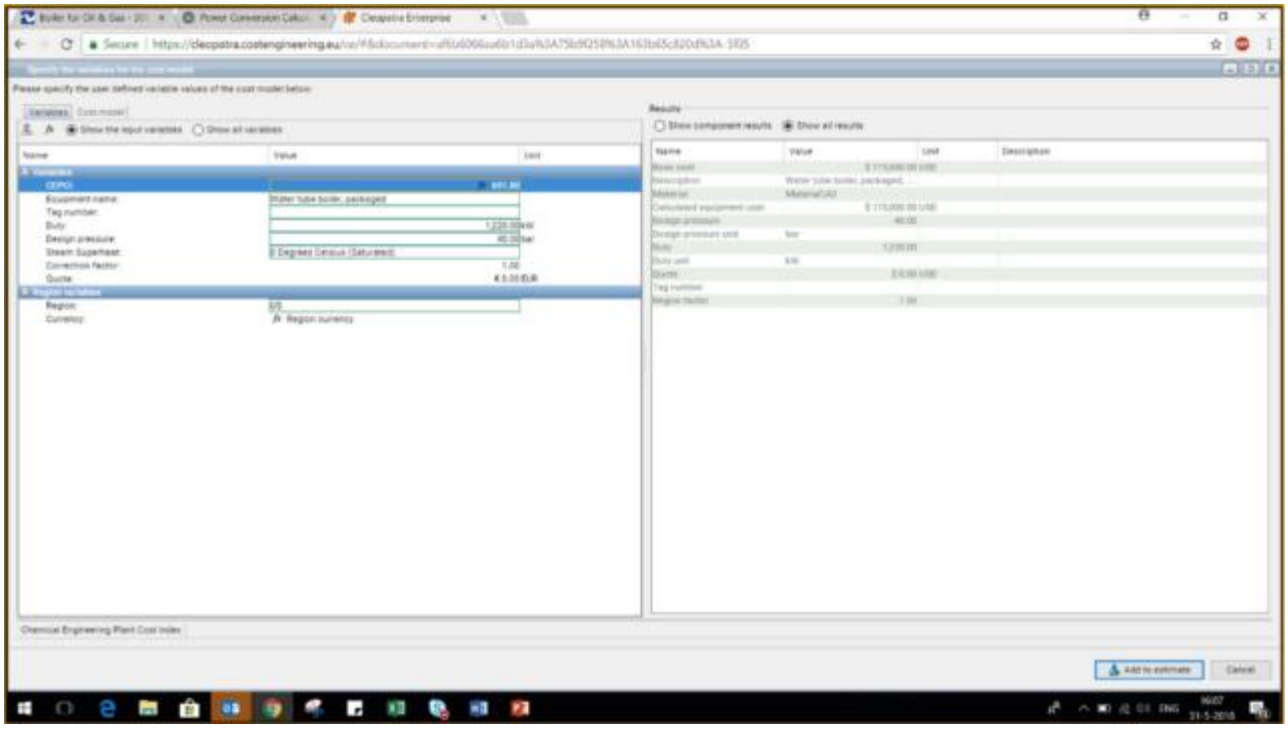
(f)

FIG. 7.4 Cont'd.



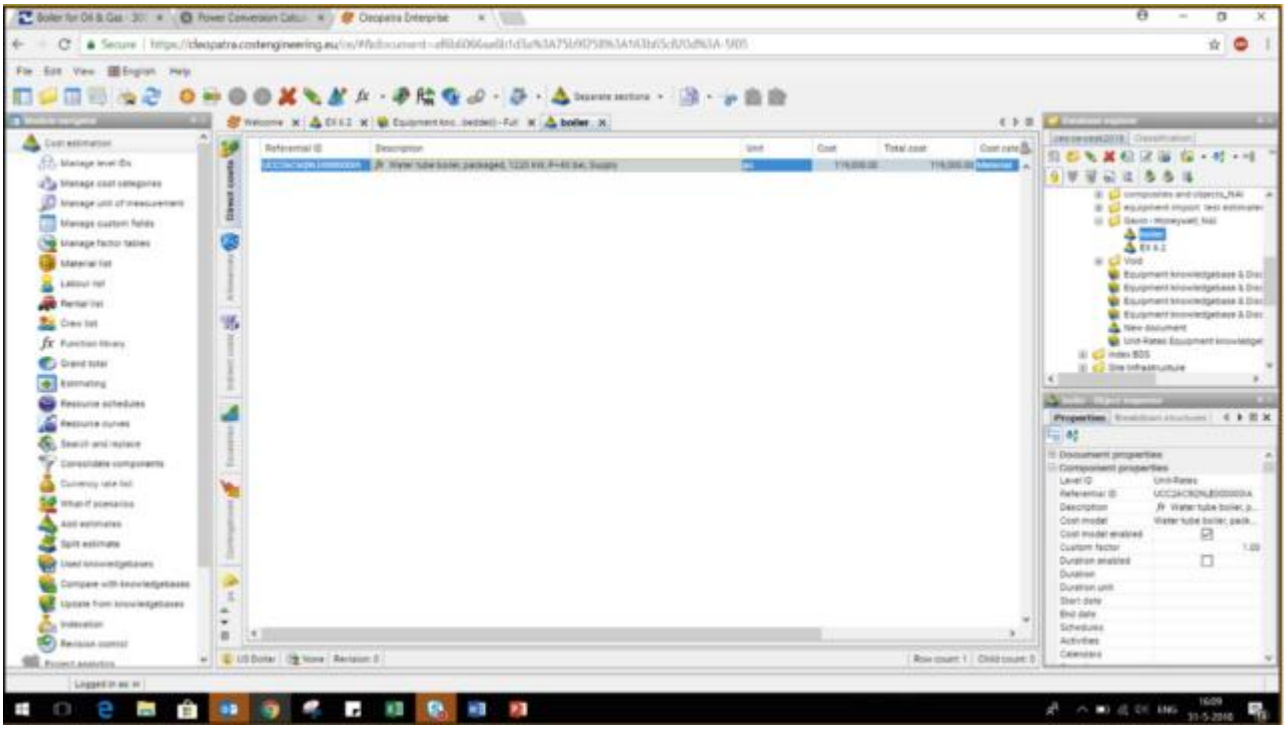
(g)

FIG. 7.4 Cont'd.



(h)

FIG. 7.4 Cont'd.



(i)

FIG. 7.4 Cont'd.

Additional resources for cost estimating are available from the various cost estimating associations: the AACE International (www.aacei.org); the Project Management Institute (www.pmi.org); the UK Association of Cost Engineers (www.acoste.org.uk); and the International Cost Engineering Council (ICEC) (www.icoste.org). The ICEC website has links to cost engineering societies in 46 countries.

Example 7.8

Adipic acid is used in the manufacture of nylon 6,6. It is made by hydrogenation of phenol to a mixture of cyclohexanol and cyclohexanone (known as *KA oil*—ketone and alcohol), followed by oxidation with nitric acid. Estimate the fixed capital cost for a 400,000 metric ton per year (400 kMTA) adipic acid plant located in northeast Asia in 2020.

Solution

The capital cost of the process can be estimated based on historic data using the correlation given in Table 7.1. The correlation is based on the plant capacity in MMlb/y, so we need to convert the capacity: 400 kMTA is equal to 880 MMlb/y:

$$\text{ISBL capital cost} = 3.533\, S^{0.6} = 3.533(880)^{0.6} = \$206.5 \text{ MM}$$

The ISBL cost is on a 2006 U.S. Gulf Coast basis, so we need to convert to a 2020 northeast Asia basis. If we look up the location factor in Table 7.7, it is not clear what factor we should use. The location factor for Japan is 1.26, whereas for China it varies from 0.6 to 1.1, depending on the amount of indigenous vs. imported equipment used. Because the exact location of the plant has not yet been specified, we are not able to make a definitive assessment of what the location factor should be. As a first approximation we therefore assume it is 1.0 and note that this should be revisited as part of the sensitivity analysis.

The OSBL capital cost is estimated as 40% of ISBL cost. The engineering cost and contingency are estimated as 10% and 15% of the sum (ISBL + OSBL) cost, respectively, giving a total fixed capital cost on a 2006 basis of $361.3 MM.

Note that this cost is on a January 2006 basis, as that was the basis of the correlation in Table 7.1. We can update this to a 2020 basis using the CEPCI index. From Fig. 7.2 (or by looking up the index in *Chemical Engineering*):

$$\text{Index in 2006} = 499.6$$

Index for full year 2020 is not yet known, but is likely to be in the range of 570 to 600,

so as a conservative estimate we can assume Index in 2020 = 600.

$$\text{So, estimated total fixed capital cost in 2020} = \$361.3 \text{ MM} \times 600/499.6 = \underline{\underline{\$433.9 \text{ MM}}}.$$

The impact of updating this estimate is further explored in Problems 7.9 and 9.6.

7.12 References

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7.13 Nomenclature

		Dimensions in $MLTθ
A	Area	$\mathbf{L^2}$
a	Constant	**$**
b	Constant	**$**
C	Capital cost	**$**
C_e	Purchased equipment cost	**$**
$C_{e,i,A}$	Purchased cost of equipment i in alloy	**$**
$C_{e,i,CS}$	Purchased cost of equipment i in carbon steel	**$**
C_1	Capital cost of plant with capacity S_1	**$**
C_2	Capital cost of plant with capacity S_2	**$**
D_c	Diameter of distillation column	**L**
D_f	Flange diameter	**L**
D_n	Nozzle diameter	**L**

Continued

		Dimensions in $MLT\theta$
D_s	Shell diameter	**L**
F	Installation (Lang) factor	—
f_c	Installation factor for civil engineering work	—
f_{el}	Installation factor for electrical work	—
f_{er}	Installation factor for equipment erection	—
f_i	Installation factor for instrumentation and control	—
f_l	Installation factor for lagging, insulation and paint	—
f_m	Materials factor	—
f_p	Installation factor for piping	—
f_s	Installation factor for structures and buildings	—
L_c	Vessel length	**L**
L_s	Shell length	**L**
LF_A	Location factor for location A relative to U.S. Gulf Coast basis	—
M	Total number of pieces of equipment	—
N	Number of significant processing steps (functional units)	—
N_b	Number of bolts	—
N_{baf}	Number of baffles	—
N_t	Number of tubes	—
n	Capital cost exponent	—
Q	Plant capacity	$\mathbf{MT}^{-1}$
S	Plant or equipment capacity	*
S_{lower}	Lower end of capacity range over which correlation is valid	*
S_{upper}	Upper end of capacity range over which correlation is valid	*
S_1	Capacity of plant	1 *
S_2	Capacity of plant	2 *
s	Reactor conversion	—
TCOP	Total cost of production	$\mathbf{\$M^{-1}}$ or $\mathbf{\$T^{-1}}$
t	Time, project life in years	**T**
t_f	Flange thickness	**L**
t_s	Shell thickness	**L**
t_w	Vessel wall thickness	**L**
ρ	Metal density	$\mathbf{ML^{-3}}$

Asterisk (*) indicates that the dimensions are dependent on the type of equipment or process.

Acronyms

AACEI Association for the Advancement of Cost Estimating International
APC Automatic Process Control
CEPCI Chemical Engineering Plant Cost Index, published monthly in *Chemical Engineering*
EPC Engineering, Procurement and Construction
FEED Front End Engineering Design
ISBL Inside Battery Limits, referring to parts of the plant itself
MM Million (abbreviation commonly used in industry in United States)
M&S Marshall and Swift cost index, published monthly in *Chemical Engineering*
NF Nelson-Farrer refinery cost index, published monthly in *Oil and Gas Journal*
NWE Northwest Europe, often used as a location basis in capital costing
OSBL Outside Battery Limits, referring to site infrastructure, also known as off-sites
TCOP Total cost of production, including allowance for capital charges
USGC U.S. Gulf Coast, often used as a location basis in capital costing
WBS Work Breakdown Structure
WC Working Capital

7.14 Problems

7.1. Estimate the capital cost of a plant that produces 80,000 metric tons per year of caprolactam.

7.2. The process used in the manufacture of aniline from nitrobenzene is described in Appendix F, design problem F.8. The process involves six significant stages:

- Vaporization of the nitrobenzene
- Hydrogenation of the nitrobenzene
- Separation of the reactor products by condensation
- Recovery of crude aniline by distillation
- Purification of the crude nitrobenzene
- Recovery of aniline from wastewater streams
- Estimate the capital cost of a plant to produce 20,000 metric tons per year.

7.3. A reactor vessel cost $365,000 in June 1998; estimate the cost in January 2020.

7.4. The cost of a distillation column was $225,000 in early 1998; estimate the cost in January 2024.

7.5. Using the data on equipment costs given in this chapter or commercial cost estimating software, estimate the cost of the following equipment:

1. A shell and tube heat exchanger, heat transfer area 50 m^2, floating head type, carbon steel shell, stainless steel tubes, operating pressure 25 bar.
2. A kettle reboiler: heat transfer area 25 m^2, carbon steel shell and tubes, operating pressure 10 bar.
3. A horizontal, cylindrical, storage tank, 3 m diameter, 12 m long, used for liquid chlorine at 10 bar, material carbon steel.
4. A plate column: diameter 2 m, height 25 m, stainless clad vessel, 20 stainless steel sieve plates, operating pressure 5 bar.

7.6. Compare the cost of the following types of heat exchangers, each with a heat transfer area of 10 m^2. Take the construction material as carbon steel.
1. Shell and tube, fixed head.
2. Double-pipe.

7.7. Estimate the cost of the following items of equipment:

1. A packaged boiler to produce 20,000 kg/h of steam at 40 bar.
2. A centrifugal compressor, driver power 75 kW.
3. A plate and frame filter press, filtration area 10 m^2.
4. A floating roof storage tank, capacity 50,000 m^3.
5. A cone roof storage tank, capacity 35,000 m^3.

7.8. A storage tank is purged continuously with a stream of nitrogen. The purge stream leaving the tank is saturated with the product stored in the tank. A major part of the product lost in the purge could be recovered by

installing a scrubbing tower to absorb the product in a solvent. The solution from the tower could be fed to a stage in the production process and the product and solvent recovered without significant additional cost.
A preliminary design of the purge recovery system has been made. It would consist of:

1. A small tower 0.5 m diameter, 4.0 m high, packed with 25 mm ceramic saddles, packed height 3.0 m.
2. A small storage tank for the solution, 5 m^3 capacity.
3. The necessary pipe work, pump, and instrumentation.

All the equipment can be constructed from carbon steel.
Using the following data, evaluate how long it would take for the cost savings to pay for the capital cost of installing the recovery system:

1. Cost of product $5 per lb.
2. Cost of solvent $0.5 per lb.
3. Additional solvent make-up 10 kg/d.
4. Current loss of product 0.7 kg/h.
5. Anticipated recovery of product 80%.
6. Additional utility costs, negligible.

Other operating costs will be insignificant.

7.9. Example 7.8 developed the cost for an adipic acid plant on a northeast Asia January 2006 basis. Estimate the cost of the plant on a 2024 basis if the plant is located in Japan, South Korea, or China. In the case of China, assume that 85% of the plant cost can be sourced indigenously.

7.10. The production of methyl ethyl ketone (MEK) is described in Appendix F, Problem F.3. A preliminary design has been made for a plant to produce 10,000 metric tons per year (t/y). The major equipment items required are listed here. The plant operating rate will be 8000 hours per year. Estimate the capital required for this project.
The plant will be built on an existing site with adequate infrastructure to provide the ancillary requirements of the new plant (no off-site investment is needed).

Major equipment items:

1. Butanol vaporizer: shell and tube heat exchanger, kettle type, heat transfer area 15 m^2, design pressure 5 bar, material carbon steel.
2. Reactor feed heaters (two): shell and tube, fixed head, heat transfer area 25 m^2, design pressure 5 bar, material stainless steel.
3. Reactors (three): shell and tube construction, fixed tube sheets, heat transfer area 50 m^2, design pressure 5 bar, material stainless steel.
4. Condenser: shell and tube heat exchanger, fixed tube sheets, heat transfer area 25 m^2, design pressure 2 bar, material stainless steel.
5. Absorption column: packed column, diameter 0.5 m, height 6.0 m, packing height 4.5 m, packing 25 mm ceramic saddles, design pressure 2 bar, material carbon steel.
6. Extraction column: packed column, diameter 0.5 m, height 4 m, packed height 3 m, packing 25 mm stainless steel pall rings, design pressure 2 bar, material carbon steel.
7. Solvent recovery column: plate column, diameter 0.6 m, height 6 m, 10 stainless steel sieve plates, design pressure 2 bar, column material carbon steel.
8. Recovery column reboiler: thermosyphon, shell and tube, fixed tube sheets, heat transfer area 4 m^2, design pressure 2 bar, material carbon steel.
9. Recovery column condenser: double pipe, heat transfer area 1.5 m^2, design pressure 2 bar, material carbon steel.
10. Solvent cooler: double pipe exchanger, heat transfer area 2 m^2, material stainless steel.
11. Product purification column: plate column, diameter 1 m^2, height 20 m, 15 sieve plates, design pressure 2 bar, material stainless steel.
12. Product column reboiler: kettle type, heat transfer area 4 m^2, design pressure 2 bar, material stainless steel.
13. Product column condenser: shell and tube, floating head, heat transfer area 15 m^2, design pressure 2 bar, material stainless steel.
14. Feed compressor: centrifugal, rating 750 kW.
15. Butanol storage tank: cone roof, capacity 400 m^3, material carbon steel.
16. Solvent storage tank: horizontal, diameter 1.5 m, length 5 m, material carbon steel.
17. Product storage tank: cone roof, capacity 400 m^3, material carbon steel.

CHAPTER

8

Estimating revenues and production costs

KEY LEARNING OBJECTIVES

- How to evaluate the revenues and production costs associated with a project
- How to determine prices for feeds, products, by-products, and fuels
- How to estimate fixed and variable production costs
- How to forecast prices over the expected life of a project
- How to summarize production cost information in a standard form

8.1 Introduction

Estimation of the product revenues and costs of production is a key step in determining the profitability of a process. An understanding of the breakdown of production costs is critically important to process optimization, regardless of whether the project is a new grassroots design or a revamp or expansion of an existing plant.

Several companies regularly publish economic analyses of chemical processes. Nexant publishes the Process Evaluation and Research Planning (PERP) reports (www.nexant.com/products). Roughly ten new reports are issued each year, and almost 200 processes have been analyzed. The PERP reports provide estimates of capital and operating costs, usually for two or three process alternatives, as well as an overview of the current market conditions for the product. SRI publishes the Chemical Economics Handbook (CEH) series, which contains 281 reports on a range of commodity and specialty chemicals. The CEH reports provide an overview of production technologies and analyses of several regional markets but do not provide the level of production cost detail given in the PERP reports. Various consulting firms also carry out paid economic studies of "state-of-the-art" technology. Although there are minor variations in methodology, most of these studies estimate production costs using similar assumptions. The conventional terminology and assumptions used in commercial studies will be introduced in the following sections and should be followed when making preliminary economic analyses and when accurate cost information is not available.

8.2 Costs, revenues, and profits

This section introduces the components of project costs and revenues. Costs and revenues for a plant are typically expressed per unit time or per unit of production of main product. The most common measures used for chemicals and bulk materials are $/year, $/day, $/lb, and $/metric ton, but some industries use other measures, such as $/kg for high-value, small-production pharmaceutical compounds or $/bbl for oil refineries.

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8.2.1 Variable costs of production

Variable costs of production are costs that are proportional to the plant output or operation rate. These include the costs of:

1. Raw materials consumed by the process.
2. Utilities — fuel burned in process heaters, steam, cooling water, electricity, raw water, instrument air, nitrogen, and other services brought in from elsewhere on the site.
3. Consumables — solvents, acids, bases, inert materials, corrosion inhibitors, additives, catalysts, and adsorbents that require continuous or frequent replacement.
4. Effluent disposal — running costs of treating any solid, liquid, or vapor emissions or waste products from the process.
5. Packaging and shipping — drums, bags, tankers, freight charges, etc.

Variable costs are mainly determined by the choice of feedstock, process chemistry, and plant location, and can usually be reduced by more efficient design or operation of the plant. Methods for estimating variable costs are discussed in Section 8.4.

8.2.2 Fixed costs of production

Fixed production costs are costs that are incurred regardless of the plant operation rate or output. If the plant cuts back its production, these costs are not reduced. Fixed costs are discussed in more detail in Section 8.5. Fixed costs include:

1. Operating labor — see Section 8.5.1.
2. Supervision — usually taken as 25% of operating labor.
3. Direct salary overhead — usually 40% to 60% of operating labor plus supervision. These are nonsalary costs such as employee health insurance and other benefits.
4. Maintenance, which includes both materials and labor, and is typically estimated as 3% to 5% of inside battery limits (ISBL) investment, depending on the expected plant reliability. Plants with more moving equipment or more solids handling usually require higher maintenance.
5. Property taxes and insurance — typically 1% to 2% of ISBL fixed capital.
6. Rent of land (and/or buildings) — typically estimated as 1% to 2% of ISBL plus offsite battery limits (OSBL) investment. Most projects assume land is rented rather than purchased, but in some cases the land is bought and the cost is added to the fixed capital investment and recovered at the end of the plant life.
7. General plant overhead — charges to cover corporate overhead functions such as human resources, research and development (R&D), information technology, finance, etc. These costs can vary widely and are discussed in more detail in Section 8.5.6.
8. Allocated environmental charges to cover superfund payments (see Chapter 11) — typically 1% of ISBL plus OSBL cost.
9. Running license fees and royalty payments. Royalties are discussed in more detail in Section 8.5.7.
10. Capital charges — these include interest payments due on any debt or loans used to finance the project, but *do not* include expected returns on invested equity capital; see Section 9.3.
11. Sales and marketing costs — in some cases these are considered part of general plant overhead. They can vary from almost zero for some commodities to millions of dollars a year for branded items such as foods, toiletries, drugs, and cosmetics.

Fixed costs should never be neglected, even in the earliest stages of design, as they can have a significant impact on project economics. Very few chemical plants in the United States carry less than $1 million per year ($1 MM/y) of fixed costs.

Fixed costs are also a strong disincentive for building small plants. As plant size is increased, labor, supervision, and overhead costs usually do not increase, and hence the fixed cost per pound of product decreases. This, together with economies of scale in capital investment (see Section 7.4.1), gives larger plants more flexibility to reduce prices and hence force smaller plants out of business during downturns in the business cycle.

Fixed costs are not easily influenced by better design or operation of the plant, other than improvements that allow the plant to be operated safely with a smaller workforce. Fixed costs are more amenable to control at the corporate level than the plant level.

8.2.3 Revenues

The revenues for a project are the incomes earned from sales of main products and by-products.

The production rate of main product is usually specified in the design basis and is determined by the marketing department based on predictions of overall market growth.

By-product revenues

Determining which by-products to recover, purify, and sell is usually more difficult than determining the main product. Some by-products are produced by the main reaction stoichiometry, whereas others are produced from feed impurities or by nonselective reactions.

The decision to recover, purify, and sell; recycle or otherwise attenuate; or dispose of by-products as wastes is an important design optimization problem. A good deal of process design effort is often spent analyzing by-product recovery. Potentially valuable by-products include:

1. Materials produced in stoichiometric quantities by the reactions that form the main product (see Table 8.1 for examples). These stoichiometric by-products are unavoidable unless new chemistry can be found. If these are not recovered as by-products and sold for whatever price they can get, the waste disposal costs will be excessive.
2. Components that are produced in high yield by side reactions. Some examples include propylene, butylenes, and butadiene, all of which are by-products of ethylene from steam cracking of naphtha feed. Orthoxylene and metaxylene are by-products of paraxylene manufacture by catalytic reforming of naphtha.
3. Components formed in high yield from feed impurities. Most sulfur is produced as a by-product of fuels manufacture. Crude oil and natural gas contain sulfur compounds that are converted to H_2S during refining or gas treatment. The H_2S is then converted to elemental sulfur by the Claus process. Mannitol (a valuable hexose) is made from fructose that is present in the glucose feed to the sorbitol process.
4. Components produced in low yield that have high value. Dicyclopentadiene can be recovered from the products of steam naphtha cracking. Acetophenone is recovered as a by-product of phenol manufacture, although it can also be made by oxidation of ethylbenzene or fermentation of cinnamic acid.
5. Degraded consumables such as solvents that have reuse value. Spent sulfuric acid can be neutralized with calcium oxide to form low-value gypsum that is used as fill for roads. Alternatively, more expensive ammonia can be used for the neutralization, forming ammonium sulfate that has a higher by-product value as a fertilizer.

For the by-product to have value, it must meet the specifications for that material, which may entail additional processing costs. The design engineer must therefore assess whether the additional cost of recovering and purifying the by-product is justified by the by-product value and avoided waste disposal cost before deciding whether to value the material as a by-product or as a waste stream.

TABLE 8.1 Some stoichiometric by-products

Feeds	Main product	By-product
cumene + air	phenol	acetone
propylene + ethylbenzene + air	propylene oxide	styrene
ethylene + chlorine	vinyl chloride monomer	HCl
allyl chloride + HOCl + NaOH	epichlorohydrin	NaCl
methane + steam	hydrogen	carbon dioxide
glucose	ethanol (by fermentation)	carbon dioxide
acetone cyanohydrin + methanol + H_2SO_4	methyl methacrylate	ammonium sulfate
sodium chloride + electricity	chlorine	sodium hydroxide

An algorithm for assessing the economic viability of recovering a by-product X is given in Fig. 8.1. Note that it is important to consider not only the cost of purifying the by-product but also whether it can be converted into something more valuable. This would include recycling the by-product within the process if that might be expected to lead to a higher yield of main product or formation of a more valuable by-product. Note also that when analyzing whether to recover a by-product, the value created by recovering the by-product includes not only the revenue from by-product sales but also the avoided by-product disposal cost. If the by-product has fuel value, the fuel value should be subtracted from the revenue instead.

A rule of thumb that can be used for preliminary screening of by-products for large plants is that for by-product recovery to be economically viable, the net benefit must be greater than $200,000 per year. The net benefit is the by-product revenue plus the avoided waste disposal cost. (This rule of thumb is based on the assumption that recovering by-product is going to add at least one separation to the process, which will cost at least $0.5MM of capital, or an annualized cost of about $170,000, as described in Section 9.7.2.).

8.2.4 Margins and profits

Margins

The sum of product and by-product revenues minus raw material costs is known as the gross margin (or sometimes product margin or just margin).

$$\text{Gross margin} = \text{Revenues} - \text{Raw materials costs} \tag{8.1}$$

Gross margin is a useful concept, as raw materials costs are almost always the largest contributor to production costs (typically 80% to 90% of total cost of production). Raw materials and product prices of commodities are often subject to high variability and can be difficult to forecast, but margins suffer less variability if producers are able to pass feedstock price increases on to their customers. Margins are therefore often used in price forecasting, as described in Section 8.3.3.

Note that the gross margin is based on the actual amount of raw materials consumed and is not simply the product price per ton minus the feed price per ton. This is a common source of confusion.

Margins vary widely between different sectors of the chemical industry. For commodities such as bulk petrochemicals and fuels, margins are typically very low (less than 10% of revenues) and may even occasionally be negative. Commodity businesses are usually cyclical because of investment cycles and experience higher margins when supply is short, as described in Section 8.3.1. When a product is tightly regulated (making market entry difficult) or subject to patent protection, then margins can be much higher. For example, margins on food additives, pharmaceutical products, and biomedical implants are typically more than 40% of revenues and often higher than 80% of revenues.

The variable contribution margin is the sum of revenues minus variable costs:

$$\text{Variable contribution margin} = \text{Revenues} - \text{Variable costs of production} \tag{8.2}$$

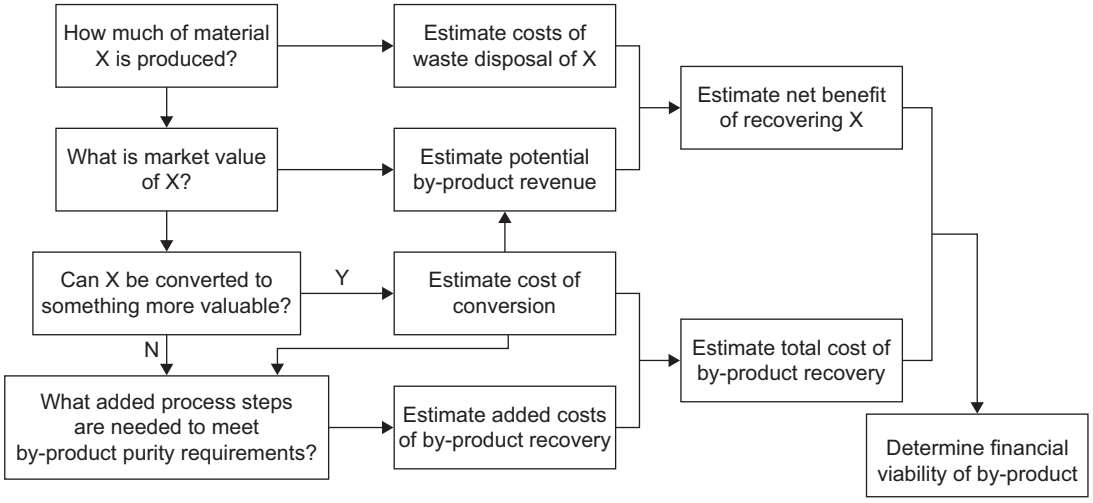


FIG. 8.1 Algorithm for assessing the economic viability of by-product recovery.

Variable contribution margin indicates the profitability of the process on a fixed-cost-free basis. It is often used in batch processing when assessing the impact of adding a new product to an existing plant that is not fully utilized, so that the new product can be accommodated without increasing fixed costs.

Profits

The cash cost of production (CCOP) is the sum of the fixed and variable production costs:

$$\text{CCOP} = \text{VCOP} + \text{FCOP} \tag{8.3}$$

where VCOP = sum of all the variable costs of production minus by-product revenues
FCOP = sum of the fixed costs of production

The CCOP is the cost of making a product, not including any return on the equity capital invested. By convention, by-product revenues are usually taken as a credit and included in the VCOP. This makes it easier to determine the $/lb cost of producing the main product.

The gross profit is:

$$\text{Gross profit} = \text{Main product revenues} - \text{CCOP} \tag{8.4}$$

Gross profit should not be confused with gross margin, as gross profit includes all the other variable costs in addition to raw materials and also includes fixed costs and by-product revenues.

In some companies gross profit is stated on a plant basis, omitting the general overhead charges and selling costs (selling, general, and administrative, or SG&A, charges: items 7 and 11 in the list of fixed costs in Section 8.2.2). The SG&A charges are then subtracted from the gross profit at the corporate level to give the operating income reported in the annual income statement.

The profit made by the plant is usually subject to taxation. Different tax codes apply in different countries and locations, and the taxable income may not be the full gross profit. Taxes are discussed in more detail in Section 9.4. The net profit (or cash flow after tax) is the amount left after taxes are paid:

$$\text{Net profit} = \text{gross profit} - \text{taxes} \tag{8.5}$$

The net profit from the project is the money that is available as a return on the initial investments. Methods for evaluating the economic performance of investments are introduced in Chapter 9.

It is sometimes useful to calculate a total cost of production (TCOP), assuming that a plant generates a specified return on investment. In this case, an annual capital charge (ACC) is added to the cash cost of production:

$$\text{TCOP} = \text{CCOP} + \text{ACC} \tag{8.6}$$

Methods for calculating the annual capital charge are discussed in Section 9.7.

8.3 Product and raw material prices

The revenues and variable costs of production are obtained by multiplying the product, feed, or utility flow rates from the flowsheet by the appropriate prices. The difficult step is usually finding good price data. The prices used in economic analysis of a design should reflect the market conditions that the company expects to face over the life of the project. It is therefore necessary to make a long-term forecast of prices. This section discusses the factors that influence prices, where to obtain historic price data, and how to use that data to make forecasts of future prices for use in economic analysis.

The chemical and process industries handle a very broad range of materials, ranging from bulk commodities such as crude oil, naphtha, grains, and basic chemicals to specialized products such as drugs, food additives, scents, and biologically derived molecules. Some of the most basic materials are traded on commodity exchanges, and their price can fluctuate significantly on a daily or even hourly basis. Materials that are supplied in large bulk quantities are usually sold under long-term contracts. The contract price may be pegged to the price of a commodity such as natural gas, corn, or crude oil, or may be subject to periodic renegotiation, typically on a quarterly or annual basis. Materials that are supplied in smaller quantities have a list price specified by the supplier, but the actual price paid by a purchaser is usually the result of a negotiation between the purchaser's procurement department and the supplier's sales department and can depend on the quantity purchased, delivery terms, and other factors. Even finished products such as household chemicals, medicines, and personal care products that are ready for sale to

end users are not immune from price negotiation, as large retailers typically use their control of sales volume to exert price pressure on their suppliers. Companies like Walmart, Costco, and Target can extract significant price concessions from chemicals manufacturers, and hence maximize their own margins.

8.3.1 Pricing fundamentals

The price of any substance is determined by the balance between supply and demand; indeed, in economics the price is the mechanism used by the market to bring supply and demand into dynamic equilibrium.

As the price of any product or service decreases, more customers can afford or are willing to buy the product, and demand for the product increases. We can plot a graph of how much demand there will be for the product (i.e., the quantity that can be sold) as a function of price, which is known as a *demand curve*; Fig. 8.2(a). A demand curve can be thought of as a rank ordering of the customers in terms of the amount they will consume and their willingness to pay.

Similarly, if the price of a product or service increases, more suppliers will be attracted to enter the market, and the quantity of the product that is supplied will increase. We can make a similar plot of the marginal production of the product as a function of price, which is known as a *supply curve*; Fig. 8.2(b). A supply curve can also be thought of as a rank ordering of producers in terms of the amount they can produce and their willingness to sell.

Because the supply and demand curves both relate price to quantity, they can be plotted on the same graph, as in Fig. 8.3. The intersection of the supply and demand curves sets the equilibrium between supply and demand. The intersection point gives the transaction price at which the most marginal consumer agrees to buy and the most marginal producer agrees to sell, as well as setting the volume of the market. At any point to the right of the equilibrium point there is no supplier who can provide product at a price that the next most marginal customer is willing to pay.

The slope of the supply or demand curve is referred to as the elasticity of supply or demand. If the curve is flat and price varies very little with quantity, then the supply or demand is said to be elastic [Fig. 8.4(a)], whereas if the slope is steep and a large change in price makes little difference to demand, then the supply or demand is said to be inelastic [Fig. 8.4(b)]. The elasticity of demand depends on the availability of substitutes, the amount of money

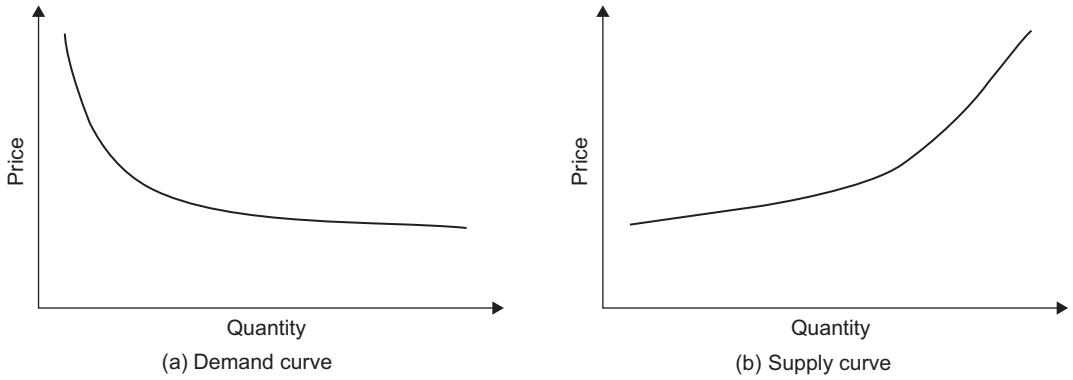


FIG. 8.2 Demand and supply curves.

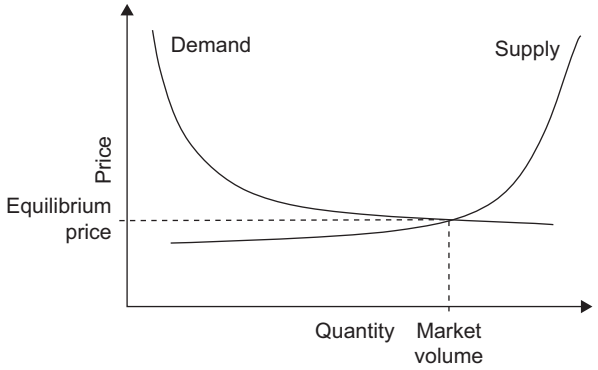


FIG. 8.3 Market equilibrium.

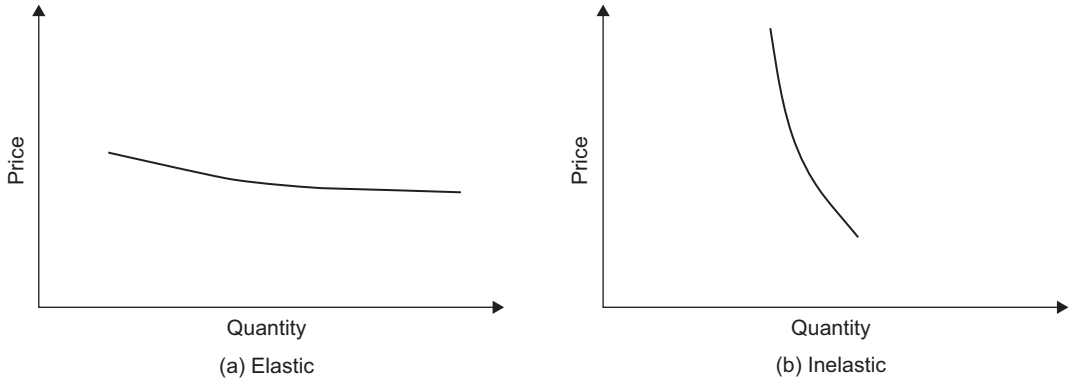


FIG. 8.4 Elasticity of demand.

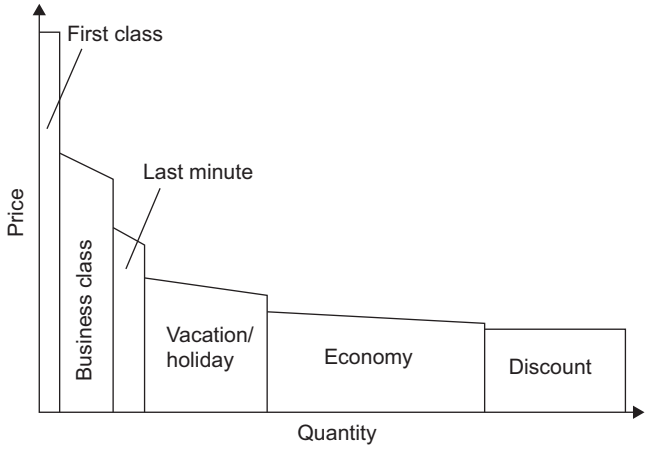


FIG. 8.5 Demand segmentation for air travel.

available to consumers, and the consumers' perception of the marginal utility or value of the product or service. The elasticity of supply depends on how many producers are able to produce an equivalent product or service, how difficult it is to enter the market, and producers' perception of the marginal value of the product or service.

There are several methods that companies can use to maximize the price that they obtain for their products or services. One of the most straightforward is to offer products of different quality aimed at different segments of the market. Each product has its own intersection point on the demand curve and hence can have a different price. For example, Fig. 8.5 is a schematic demand curve for airline travel. By segmenting the customers according to need to travel and willingness to pay, an airline can develop a pricing structure that commands substantial premiums for offering essentially the same service of moving a person from city A to city B. Another familiar example of market segmentation is the garment industry, where retailers develop brands aimed at different demographics so as to maximize the price commanded for relatively small differences in product quality.

Technology and new products can also be used to create barriers to entry into a market and capture a higher price from a defined customer segment. New technologies are generally launched in relatively small quantity at high price, as patent holders are able to control the supply of the product. As patents expire and competitors emerge, the supply increases and price decreases. Products therefore tend to move down the demand curve from left to right with time. Many pharmaceutical products undergo a substantial drop in price when their patents expire, as generic manufacturers are then able to enter the market and increase the supply.

If a supplier gains a monopoly of supply or if a group of suppliers form a cartel, then they can restrict supply and use this as a means of raising prices. In this case, the supply is constrained to a value that corresponds to the target price sought by the suppliers. International trade, competition, and antitrust laws prohibit cartels and impose fines on companies that engage in price fixing; however, cartels tend to be unstable in any case, as there will always be the possibility that the producer can increase their income by allowing demand to grow and segmenting the market to target different consumers. There are well-publicized examples of companies that have benefited from abandoning

cartels and making better use of customer segmentation instead. For example, De Beers now has better financial performance with a 40% market share than it had when it restricted diamond supply and maintained 80% market share in the 1990s.

For chemicals, fuels, foods, and pharmaceutical products, the barriers to entry into a market can create inelasticity in supply. It usually takes several years to design, build, and commission a new chemical plant. The supply curve can be segmented in a similar manner to the demand curve. For example, Fig. 8.6 shows a hypothetical supply curve for a commodity chemical. The lowest-cost producers are typically large, efficient new plants located in regions that have advantageously priced feedstocks. Next are large, efficient plants without feedstock advantage, as these have low utility costs and utilities are usually the next largest cost after feeds. Smaller and older plants carry a higher burden of fixed costs and labor costs, so labor cost advantages are only usually significant for smaller scales of production. The most marginal older plants will be idled or mothballed if they cannot produce product at a price the market is willing to pay.

In most chemical sectors, the overall capacity utilization rate varies between about 75% and 85%, and there is sufficient spare capacity to allow for some plants to be down for maintenance or unexpected interruptions in production. The market equilibrium is therefore at a point where the supply is relatively elastic; however, if the capacity utilization rate increases to greater than 90%, the market equilibrium moves to the inelastic region of the supply curve and prices can become volatile. The market is then much more sensitive to events that cause temporary reductions in supply, such as unexpected shutdowns of large plants. If new plants cannot be brought on stream quickly, prices will spike until additional supply becomes available. This leads to boom and bust cycles, which tend to have the following pattern:

1. High prices create attractive conditions for investment. Several companies commit to building new plants or revamping old plants, adding more capacity than is needed.
2. When the new plants are commissioned, they have the latest technology, lowest cost feeds, and lowest cost of production. The new capacity needs to operate at full production to recoup its investment, so prices fall rapidly as supply increases. Overall, capacity utilization decreases as demand has not yet caught up with the new supply.
3. Lower prices force the least competitive producers to reduce production rates or close older, less efficient plants. Lower prices remove the incentive to add new capacity and cause underinvestment in new plant. A new equilibrium is reached at low price.
4. Demand eventually catches up with capacity, and utilization rates creep up. At some point the elasticity of supply is lost and prices begin to spike again, creating conditions to return to the start of the cycle.

Many commodity chemicals and fuels undergo such periodic oscillations in price. These oscillations can make it difficult to forecast prices for use in economic analysis of new projects, as discussed in the following sections.

8.3.2 Sources of price data

This section describes the most widely used sources of current and historic price data. Some pricing terminology is given in Table 8.2.

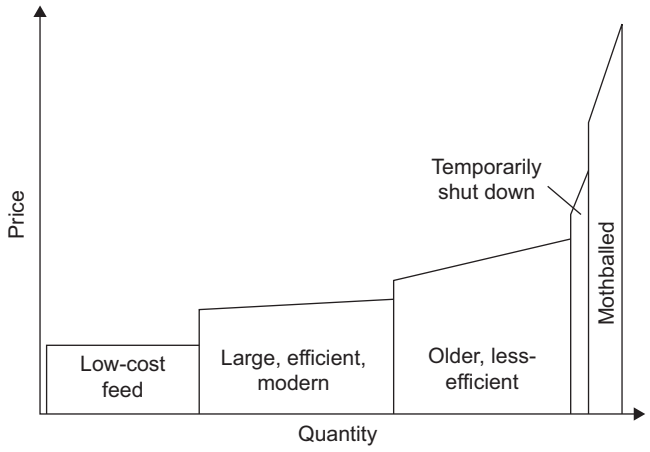


FIG. 8.6 Supply segmentation for a commodity chemical.

TABLE 8.2 Pricing terminology

Abbreviation	Meaning
c.i.f.	Cost, insurance, and freight (does not include customs charges)
dlvd.	Delivered to the end user
f.o.b.	Free on board (loaded at specified supply point, but does not include freight, insurance, or customs duties)
frt. alld.	Freight allowed (f.o.b. plus freight)
dms.	Drums
bgs.	Bags
refy.	Refinery gate
syn.	Synthetic
t.t.	Tank truck
t.c.	Tank car (rail)
t.l.	Truck load
imp.	Imported

Internal company forecasts

In many large companies the marketing or planning department develops official forecasts of prices for use in internal studies. These forecasts sometimes include multiple price scenarios, and projects must be evaluated under every scenario. Company forecasts are occasionally made available to the public. See, for example, the Shell future energy scenarios, which can be downloaded from www.Shell.com/energy-and-innovation/the-energy-future/scenarios. When an officially approved price set exists, the design engineer should use it. The main concern is then ensuring that prices for feeds, products, or consumables that are not part of the standard forecast are put on a consistent basis.

Trade journals

Several journals publish chemicals and fuel prices on a weekly basis:

ICIS Chemical Business Americas — formerly known as *Chemical Marketing Reporter* (ICIS Publications) used to list prices for 757 chemicals with multiple locations and product grades for some. This list was reduced to only 85 compounds in 2006, with most of the remaining set being natural extracts. Data for 80 chemicals, 44 fuels, and 11 base oils is now provided online through the subscription service www.icis.com. At the time of writing this service was very expensive compared with some of the other alternatives listed. ICIS also publishes *ICIS Chemical Business Europe* and *ICIS Chemical Business Asia*, which provide regional price data for a smaller set of compounds.

The *Oil and Gas Journal* (Pennwell) publishes prices for several crude oils and a range of petroleum products on U.S., northwest European, and southeast Asian bases, as well as natural gas prices for the United States. The *Oil and Gas Journal* also publishes formula estimates of gross and net margins for refineries, natural gas liquids recovery, and ethylene plants on a monthly basis.

Chemical Week (IHS) gives spot and contract prices for 22 commodity chemicals in U.S. and northwest European markets.

Consultants

There are many companies that can be hired as consultants to provide economic and marketing information or that allow access to such information on a subscription basis. The information provided generally includes market surveys and technical and economic analyses of competing technologies, as well as price data and forecasts. There is not room here to list all of these companies, but some of the most widely used are:

Purvin and Gertz: Quarterly forecasts of oil, gas, and fuels prices are widely used in the oil industry. They have a 10-year archive of historic data and forecast prices of most fuel products as well as crude oils on U.S., northwest European, Middle Eastern, and Asian bases.
Cambridge Energy Research Associates: Publishes forecasts of crude oil prices based on macroeconomics and industry trends (drilling rates, etc.).
Chemical Market Associates, Inc. (CMAI): Maintains a large archive of historic data and future price forecasts for 70 commodity chemicals, including multiple grades, U.S., northwest European, Middle Eastern, and northeast and southeast Asian. Spot and contract prices are given for some compounds, and in some cases margins are also estimated by formula.
SRI: The *Chemical Economics Handbook* series of reports published by SRI provides overviews of the markets for over 300 compounds. These reports are not updated as frequently as the others, but are useful for less commoditized compounds.

Online brokers and suppliers

A lot of price data are available online from suppliers' websites that can be found through directory sites such as www.chemicalregister.com.

Some caution is needed when using price data from the Web. The prices quoted are generally for spot sales of small-quantity orders, and are thus much higher than the market rates for large order sizes under long-term contract. The prices listed online are also often for higher-quality material such as analytical, laboratory, or United States Pharmacopeia (USP) pharmaceutical grades, which have much higher prices than bulk grades.

Reference books

Prices for some of the more common commodity chemicals are sometimes given in process economics textbooks. These prices are usually single data points rather than forecasts. They are only suitable for undergraduate design projects.

8.3.3 Forecasting prices

In most cases, it will take between 1 and 3 years for a project to go through the phases of design, procurement, and construction before the plant can begin operation. The plant will then operate for the project life of 10 to 20 years. The design engineer thus needs to carry out the economic analysis using prices forecasted over the next 20 or so years rather than the current price when the design is carried out.

For some compounds the only variation in price over time is minor adjustments to allow for inflation. This is the case for some specialty compounds that have relatively high prices and are not subject to competitive pressure (which tends to drive prices down). Prices can also be stable if they are controlled by governments, but this is increasingly rare. In most cases, however, prices are determined largely by feedstock prices, which are ultimately determined by fluctuations in the prices of commodity fuels and chemicals. The prices of these commodities are set by markets in response to variations in supply and demand, and vary widely over time.

Most price forecasts are based on an analysis of historic price data. Several methods are used, as illustrated in Fig. 8.7. The simplest method is to use the current price, Fig. 8.7(a), but this is unsatisfactory for most commodities. Linear regression of past prices is a good method for capturing long-term trends (>10 years), but can give very different results depending on the start date chosen, as shown in Fig. 8.7(b). This method can be very misleading if the data set is too small.

Many commodity prices exhibit cyclic behavior due to the investment cycle, so in some cases nonlinear models can be used, as shown in Fig. 8.7(c). Unfortunately, both the amplitude and the frequency of the price peaks usually vary somewhat erratically, making it difficult to fit the cyclic price behavior with simple wave models or even advanced Fourier transform methods.

A fourth approach, illustrated in Fig. 8.7(d) is to recognize that feed and product prices are usually closely linked, because increases in feed costs are passed on to customers whenever possible via increases in product price. Although feed and product prices may both be variable, the gross margin is subject to much less variation and can be forecasted more reliably. Forecasting of margins is the method used widely in the fuels and petrochemicals industry, as it is much easier to predict the variation in margins than the underlying variation in the prices of crude oil and natural gas. The drawbacks of this method are that it does not work so well when there are multiple routes to the same product, and it involves making assumptions about yields that may not hold true throughout the forecast period. In cases where the gross margin is high, it can be more difficult for the manufacturer to pass on the full impact of feedstock price increases in the form of increased product prices. In such cases, when feed prices rise rapidly, there is a drop in margins while producers wait for the market to absorb the impact of higher prices.

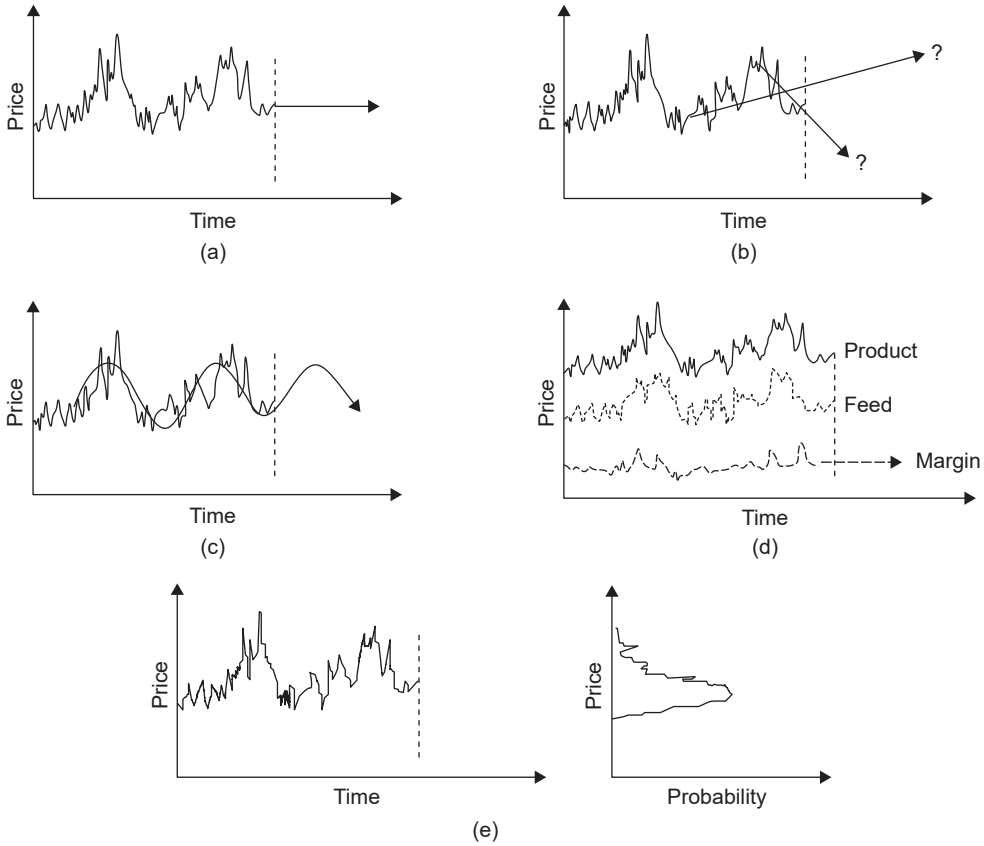


FIG. 8.7 Forecasting commodity prices.

Another method is to model the statistical distribution of the price (or margin), as illustrated in Fig. 8.7 (e). At its simplest, this method involves taking the average price, adjusted for inflation, over a recent period. This method can miss long-term trends in the data, and few prices follow any of the more commonly used distributions. It is, however, useful in combination with sensitivity analysis methods such as Monte Carlo simulation (see Section 9.8.3).

Fig. 8.8 shows North American prices from CMAI data for polyethylene terephthalate resin (PET), which is made from terephthalic acid (TPA), which in turn is made from paraxylene (PX). Several things are apparent from Fig. 8.8:

1. The spot prices of PX and TPA show more volatility than the contract prices, as would be expected.
2. All the prices follow the same broad trends, with a major peak in 1995 and long recovery leading to a second peak in 2006–2008.
3. The sharp peak in PX spot price in 1995 was not passed on to the other prices.

Fig. 8.9 shows the simple margins for TPA-PX and PET-PX over the same period, all based on contract prices. The degree of variation in margins is clearly less than the variation in the base prices. There also appears to be a long-term decline in both TPA and PET margins relative to PX in North America.

A similar examination of feed and product prices along the value chain of a given chemical can usually provide valuable insights into the best method of forecasting. No method is perfect, and anyone capable of accurately predicting commodity prices would be well advised to pursue a more lucrative career than chemical engineering. For process design purposes, it is usually sufficient to show that the prices used for optimization and economic analysis are realistic and consistent with consensus views of the market.

8.3.4 Transfer pricing

If the raw material for plant B is the product of plant A on the same site and owned by the same company, then the price that plant B pays to plant A is known as a *transfer price*. Whenever realistic, transfer prices should be set by open market prices. This reflects the reality that plant A could sell its product on the open market or plant B could similarly buy its feed. Some cases when transfer prices do not match market prices include:

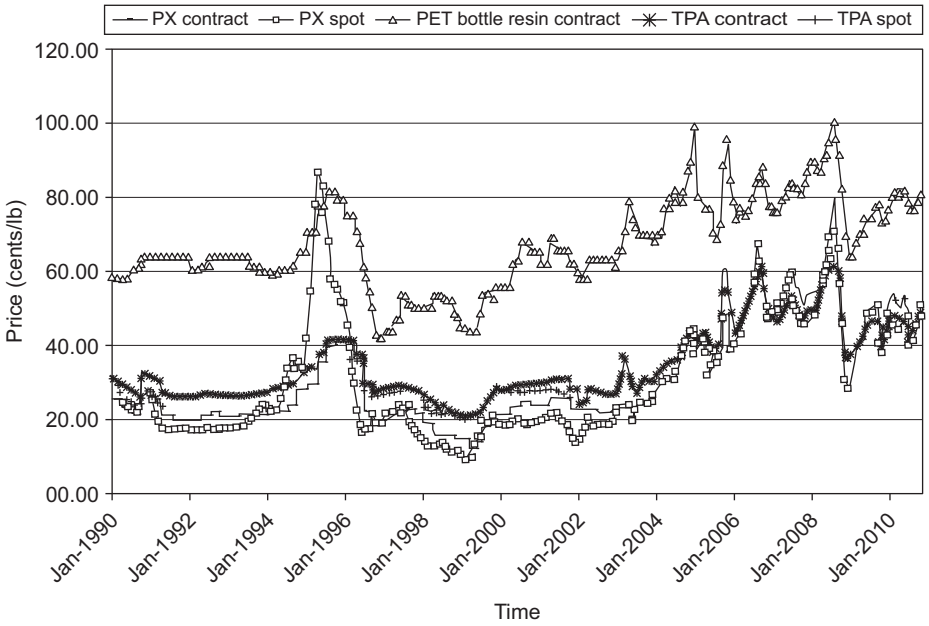


FIG. 8.8 North American prices for the PET value chain.

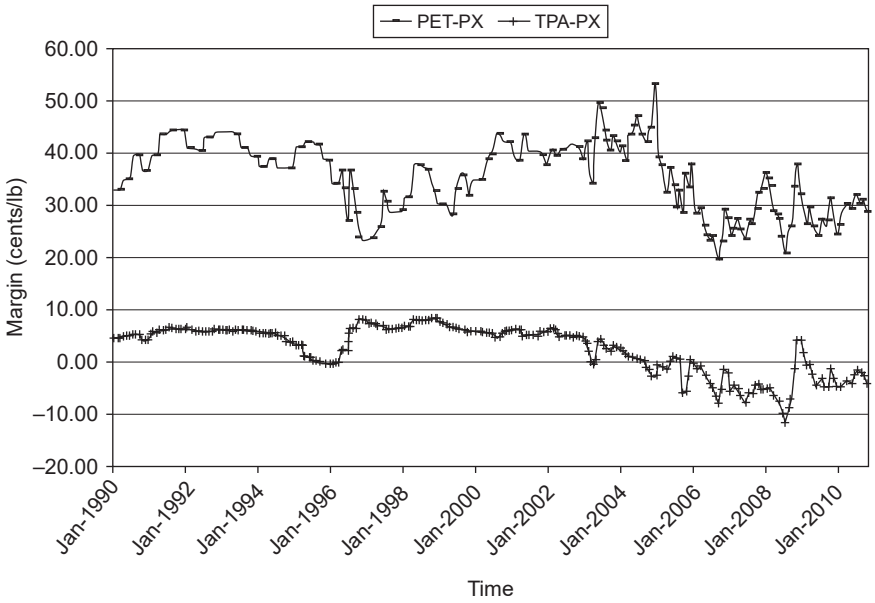


FIG. 8.9 Simple margins for the PET value chain.

1. When plant A produces material that is suitable for internal consumption but does not meet specifications for traded product. In this case, the transfer price to plant B should be discounted to allow for the added costs incurred in plant B from handling the less pure feed.
2. When plant A is underutilized or cannot sell its product and has recovered all of its initial capital investment, then the transfer price to plant B can be set at the cash cost of production of plant A (see Section 8.2.4).
3. When the pricing of product from the upstream plant is set to drive capacity utilization or conservation, for example, by using a sliding price scale based on the amount of material used.

When transfer pricing is used, it is important to keep in mind which processes actually bring in money from customers and which do not. If unrealistic transfer prices are used, uneconomic projects may seem attractive and poor investment decisions may be made.

Example 8.1

Develop forecasts for the PET-PX margin based on contract pricing using data from (a) Jan. 2000–Oct. 2010, (b) Jan. 2006–Oct. 2010, and (c) Oct. 2009–Oct. 2010. In each case, predict the PET-PX margin in Jan. 2020. Which forecast appears to be most reasonable?

Solution

The forecasts are easily constructed in Microsoft Excel using the data that were used to generate Fig. 8.9. We can make several forecasts from each data set. The simplest forecast of margins would be to assume the margin remains constant at the average value over each time period. This method gives the following results:

Time period	Average margin (cents/lb)
Jan. 2000–Oct. 2010	34.6
Jan. 2006–Oct. 2010	27.8
Oct. 2009–Oct. 2010	27.4

If margins are assumed to remain constant at the average value, then these would be the forecast predictions for Jan. 2020 margins.

Alternatively, we can make a linear regression through the data and see if there is any trend in margins with time. The results are plotted against the data sets for each time period in Figs. 8.10(a), (b), and (c).

None of the correlations are particularly good (R^2 values of 0.50, 0.09, and 0.22, respectively), although case (a) is technically the best correlation. Substituting into the fitted linear regression equations gives the following results for Jan. 2020 margins:

Time period	Linear regression forecast of Jan. 2020 margin (cents/lb)
Jan. 2000–Oct. 2010	10.4
Jan. 2006–Oct. 2010	37.3
Oct. 2009–Oct. 2010	61.6

Looking at Figs. 8.10(a) and 8.9, it seems unreasonable to believe that PET-PX margins will go as low as 10¢/lb or as high as 60¢/lb, which illustrates the difficulty in extrapolating forecasts based on linear trends. The middle forecast had the lowest correlation coefficient, but appears to yield the most reasonable value for the Jan. 2020 margin when viewed in the context of the historic data.

The final method we can consider is to look at the distribution of the data. Fig. 8.11 shows histograms of the data in each time period. For case (a), the data set appears to be bimodal, which inspection of Fig. 8.10(a) reveals to be due to an apparent step-change decrease in margins during 2005. For case (b) the data are approximately normally distributed, whereas the data set for case (c) is too small to give a good distribution.

After looking at the distributions it would seem imprudent to assume that margins would be restored to the levels they enjoyed before 2006, so we can eliminate data set (a). We can also eliminate data set (c) as being too small, so data set (b) is most suitable for a more detailed statistical analysis. For this data set we have an average value of 27.8¢/lb and a standard deviation of 3.8¢/lb. We have 98% confidence that the margin will be within ±2.05 standard deviations of the mean, so the 98% confidence interval for the 2020 forecast, assuming no time trend in the data, would be from 20.0¢/lb (= 27.8 − 7.8) to 35.6¢/lb (= 27.8 + 7.8). Note that the forecast predicted by linear regression of the time trend in the same data set lies outside this 98% confidence interval.

Regardless of the level of analysis carried out, none of the forecasts presented is clearly the best. We have no numerical basis to determine whether to believe the downward trend in margins seen during 2000–2010 or the slight upward trend experienced during 2006–2010 or the stronger upward trend during 2009–2010. A marketing group that had experience of the business conditions in this market might have supporting evidence that would bias them towards any of these positions. It would also be just as effective to look at the data in Fig. 8.9 or Fig. 8.10(a) and predict that the PET-PX margin is likely to be about 30¢/lb ± 10¢.

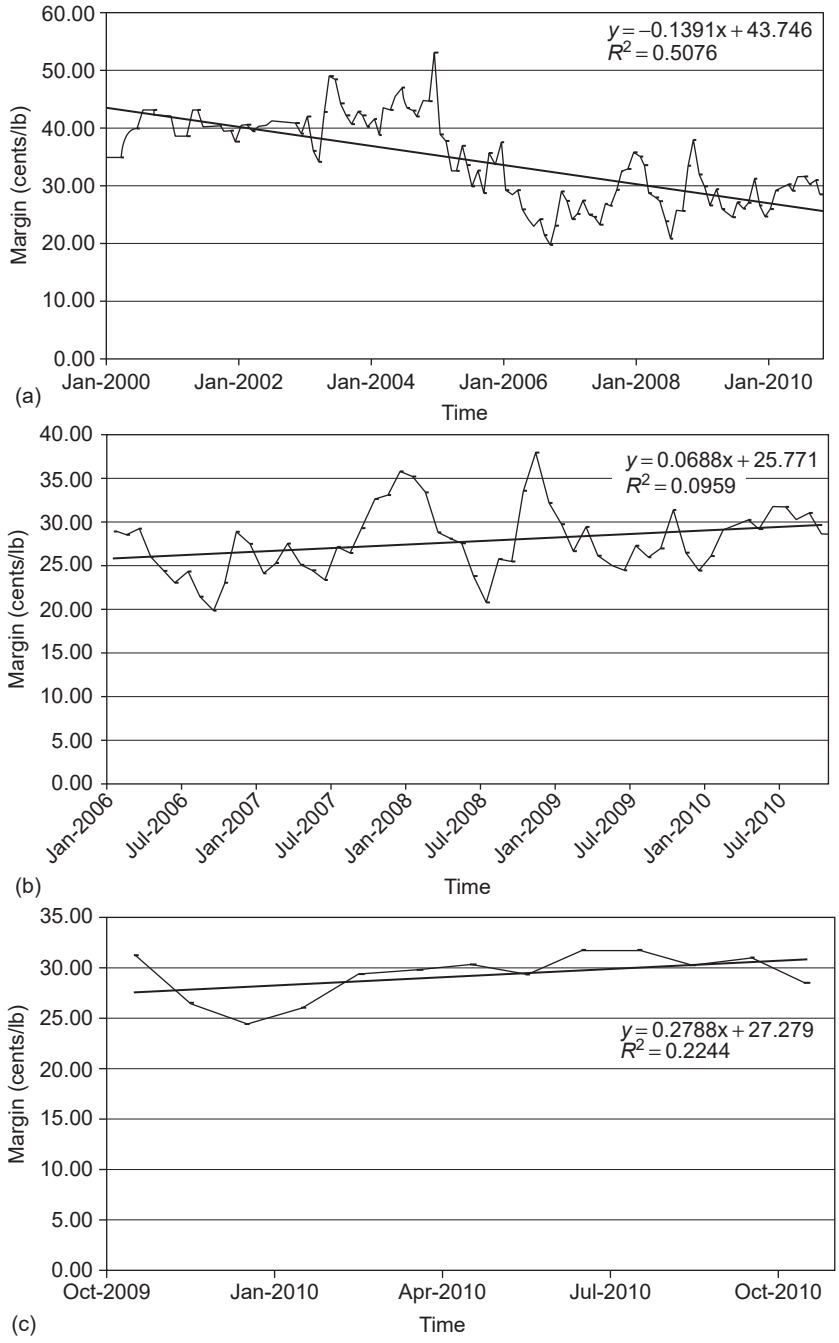


FIG. 8.10 (a) Forecast of PET-PX margins using data from Jan. 2000 to Oct. 2010. (b) Forecast of PET-PX margins using data from Jan. 2006 to Oct. 2010. (c) Forecast of PET-PX margins using data from Oct. 2009 to Oct. 2010.

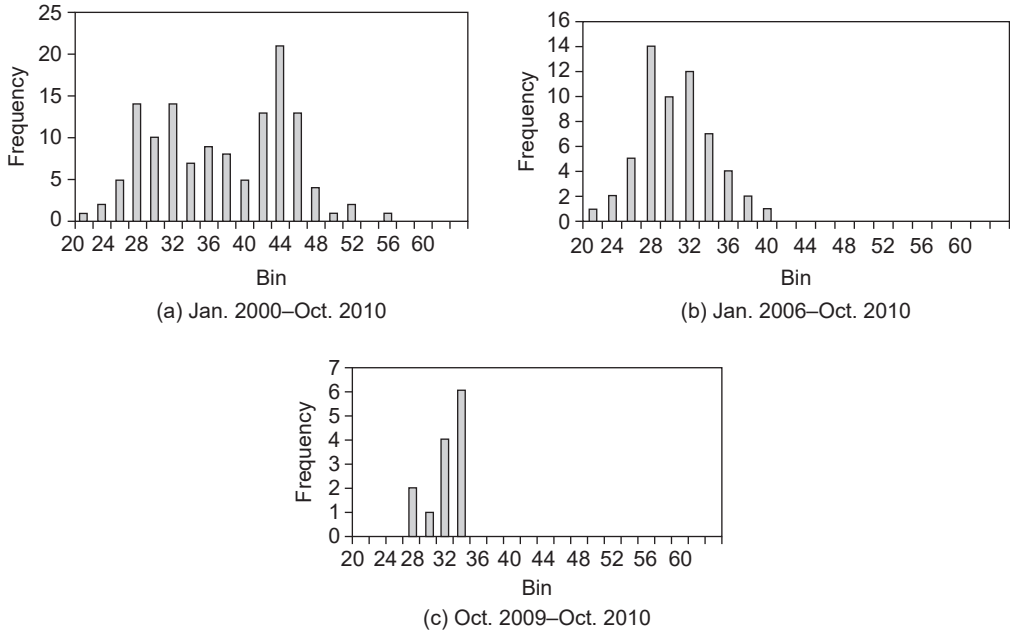


FIG. 8.11 Histograms of PET-PX margin data.

8.4 Estimating variable production costs

Variable costs of production were introduced in Section 8.2.1 and are those production costs that are directly proportional to the rate of production. For most chemicals, the major variable costs are the costs of raw materials and utilities.

8.4.1 Raw materials costs

The annual cost of each raw material is just the annual consumption multiplied by the price. Raw materials prices can be found and forecasted using the sources and methods introduced in Section 8.3.

For an existing plant, the amount of raw materials consumed per kg or lb of product can easily be determined from the plant purchasing records. One of the first steps in a revamp design is usually to assess the actual consumption to see if it is substantially different from what would be expected based on process stoichiometry and expected selectivities. Understanding any offset between the expected and actual raw material consumption can provide insights into how the process should be modified to become more efficient.

In a new design, the amount of raw materials needed to make the desired product is usually estimated using a process model to determine the overall plant material balance; see Chapter 4. Whenever possible, the process model should be benchmarked against an existing plant or pilot plant. Methods for estimating raw material consumption in the early stages of process design, when detailed models are not available, are given in Section 2.6.

Raw materials costs are typically the main contributor to overall cost of production. For most bulk chemicals and petrochemicals, raw materials costs will represent 80% to 90% of the CCOP. For specialty chemicals, raw materials costs can be as much as 95% of the CCOP. Raw materials costs are only low as a fraction of CCOP for processes that recycle waste materials or have very inexpensive feeds such as air or stranded natural gas.

8.4.2 Utilities costs

Plant utilities include fuel, process steam, cooling water, other heating or cooling fluids, electricity, process water, nitrogen, instrument air, and other service streams. Utility streams are described in detail in Section 3.2, and methods are given for determining the cost of each utility. Most utility costs are based on the cost of fuel (typically natural gas) and electricity.

Determination of process utility costs is much more difficult than determination of raw materials costs, although utilities are usually less than 15% of the CCOP and are typically about 5% to 10% of CCOP. The use of energy recovery and heat integration methods means that determination of the utility consumption of a proposed design requires not only a completed mass and energy balance of the process but also at least a preliminary design of the heat recovery network (see Sections 3.3 and 3.5).

The cost of providing heat to a process is often reduced by using process waste streams as fuel. The recovery of heat from combustion of process wastes is discussed in more detail in Section 3.4. When waste streams are used as fuel, there is a double benefit, as fuel costs are reduced and waste-handling costs are eliminated.

8.4.3 Consumables costs

Consumables include materials such as acids, bases, sorbents, solvents, and catalysts that are used in the process. Over time these become depleted or degraded and require replacement. In some cases a continuous purge and make-up is used (for example, for acids and bases), whereas in other cases an entire batch is periodically replaced (for example, sorbents, chromatography media, and catalysts).

The prices of acids, bases, and solvents can be found from the same sources used for raw materials prices. Whenever possible, the cheapest base (NaOH) or acid (H_2SO_4) would be used in the process, but for neutralizing spent sulfuric acid, lime (CaO) or ammonia (NH_3) is often used, as these bases react with sulfuric acid to form insoluble sulfates that can be recovered and sold as by-products. The cost of the process acid or base must always include the costs of neutralizing the spent stream.

The price of adsorbents and catalysts varies very widely depending on the nature of the material. The cheapest catalysts and adsorbents cost less than \$1/lb, whereas more expensive catalysts containing noble metals such as platinum and palladium have costs that are mainly determined by the amount of precious metal on the catalyst. In some cases, the value of the noble metal on a load of catalyst is so high that the chemical plant rents the catalyst rather than buying it, and when the catalyst is spent it is returned to the manufacturer for precious metal recovery.

Although small in quantity and typically costing less than 3% of CCOP, consumables can add a lot of capital cost and complexity to a plant. The plant must be designed with systems for handling, storing, metering, and disposing of all the consumables used. In many chemicals plants over half of the total pieces of equipment are associated with consumables handling.

8.4.4 Waste disposal costs

Materials produced by the process that cannot be recycled or sold as by-products must be disposed of as waste. In some cases additional treatment is required to concentrate the waste stream before sending it to final disposal.

Hydrocarbon waste streams such as off-spec products, slop oils, spent solvents, and off-gases (including hydrogen-rich gases) can often be incinerated or used as process fuel; see Section 3.4. This allows the fuel value of the stream to be recovered, and the waste stream can be assigned a value based on its heat of combustion:

$$P_{WFV} = P_F \times \Delta H_C^o \tag{8.7}$$

where: P_{WFV} = waste value as fuel (\$/lb or \$/kg)
P_F = price of fuel displaced by burning waste (\$/MMBtu or \$/GJ)
ΔH°_C = heat of combustion (MMBtu/lb or GJ/kg)

If additional systems such as flue gas scrubbers must be fitted to allow the waste to be combusted, then the waste stream value should be discounted to recover the extra cost.

Dilute aqueous streams are sent to wastewater treatment unless the contaminants are toxic to the bacteria in the wastewater plant. Acidic or basic wastes are neutralized before treatment. Neutralization is usually carried out using a base or acid that will form a solid salt that can be precipitated from the water, so that the total dissolved solids (TDS) load on the wastewater plant is not excessive. The cost of wastewater treatment is typically about \$6 per 1000 gal (\$1.5 per metric ton), but there may also be local charges for spent water discharge.

Inert solid wastes can be sent to landfills at a cost of about \$50/ton, or in some cases used to make roads. Wastes from neutralizing spent sulfuric acid are typically calcium sulfate (gypsum) that can be used as road fill, or ammonium sulfate, which can be sold as fertilizer.

Concentrated liquid streams that cannot be incinerated locally (for example, compounds containing halogens) and noninert solids must be disposed of as hazardous waste. This entails shipping the material to a hazardous waste

company for incineration in a specialized plant or long-term storage in a suitable facility. The costs of hazardous waste disposal depend strongly on the plant location, proximity to waste disposal plants, and the nature of the hazardous waste, and must be evaluated on a case-by-case basis.

Additional information on waste disposal considerations is given in Chapter 11.

8.5 Estimating fixed production costs

Fixed production costs are those costs that do not vary with the rate of production. Fixed costs include labor, maintenance, and overhead charges as well as taxes. Some finance charges are also counted as fixed costs, as described in the following sections.

8.5.1 Labor costs

The wages paid to plant operators and supervisors are treated as a fixed cost of production for almost all chemicals plants, because plant operation requires experience and safety training and it is not practical to ramp the workforce up and down with short-term changes in demand. Almost all plants are operated on a shift-work basis (even batch plants), with typically 4.8 operators per shift position. This gives a four-shift rotation with allowance for weekends, vacations and holidays, and some use of overtime. Most plants require at least three shift positions: one operator in the control room, one outside, and one in the tank farm or other feed/product shipping and receiving area. Plants that use more mechanical equipment, particularly solids-handling plants, typically require more shift positions. More shift positions are also needed when handling highly toxic compounds. In some cases two or more smaller plants may be grouped together with a common control room and tank farm to reduce the number of operators needed. Very few plants run entirely unattended, though, with the exception of gas processing plants, which hold no inventories of feed or product and are usually automated to allow a single control room operator to watch over several plants. A chart for estimating the minimum number of shift positions is given in Fig. 8.12, but it should be emphasized that this only gives a rough guide. The design engineer should always carefully think through the operations required per shift, particularly for processes that handle solids or involve batch operations or frequent sampling.

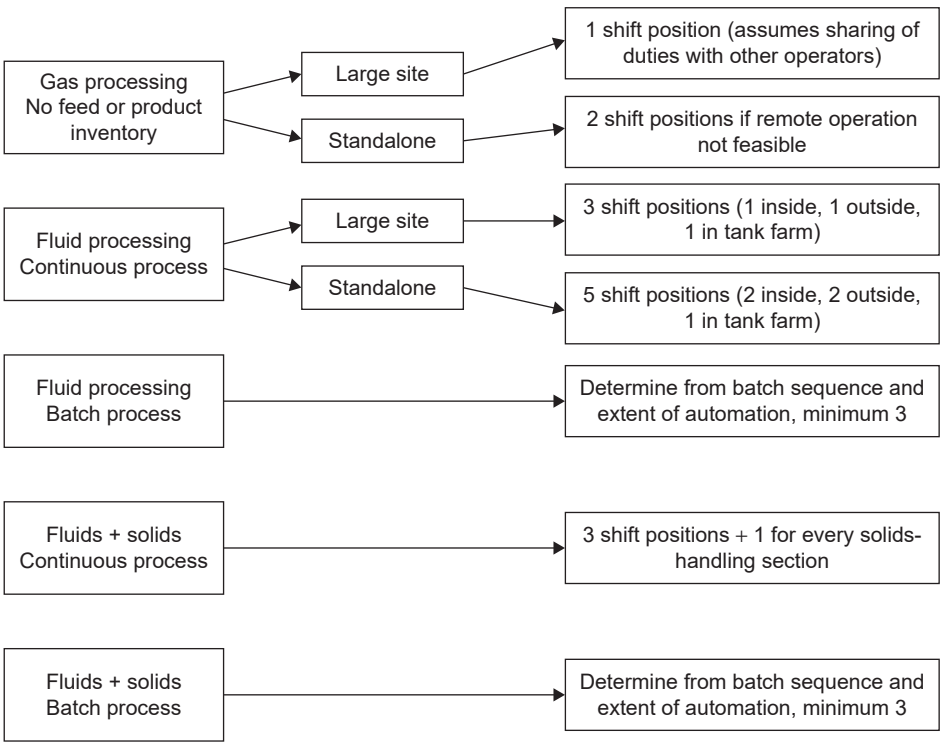


FIG. 8.12 Algorithm for assessing the minimum number of shift positions.

Operator salaries vary by region and experience level. For initial estimates, an average United States Gulf Coast (USGC) salary of $50,000 per shift position per year, not including overhead, can be used.

Supervision and management costs are typically taken as 25% of operating labor. The actual level of supervision required depends on the extent of the plant or site. In some cases, one shift supervisor can cover several plants.

Direct salary overhead costs are the costs of providing employee benefits and training. These include such nonsalary costs as health insurance, 401k contributions to employee savings plans, training courses, and benefits such as subscriptions and professional society memberships. The level of nonsalary benefits varies widely between sectors and companies, as some companies use benefits packages as a way to attract and retain employees, whereas others place more emphasis on salary alone. For example, historically the oil industry has offered relatively high salaries and low benefits, whereas the pharmaceutical industry paid lower salaries for the same experience level but offered more benefits. Direct salary overhead typically varies between 40% and 60% of labor plus supervision costs.

8.5.2 Maintenance costs

Maintenance is a fixed cost, as the plant must be kept in good repair regardless of the level of production. Operating at less than full capacity can actually increase the rate of maintenance expenditure, as damage to plant equipment is more likely during start-up, shut-down, or turndown than during steady-state operation at design capacity.

Maintenance costs include the cost of replacing or repairing parts and equipment, as well as the cost of labor needed to carry out the maintenance work. Until as recently as the 1990s, many chemical companies employed a large number of trained maintenance technicians to provide maintenance services. Over the past two decades it has become more common for companies to subcontract major maintenance overhauls and keep just a few skilled maintenance workers on site to handle day-to-day repairs.

Annual maintenance costs are typically estimated as a fraction of ISBL investment, ranging from 3%/y for a process that handles liquids and gases to 5%/y for a process that involves solids handling or other large mechanical equipment. If a process is known to require regular equipment replacement, the design engineer should make an estimate of the annualized replacement cost (see Section 9.7.2 and Example 9.6) and add this to the maintenance costs. This is the case when the designer expects the process metallurgy to cause some plant items to have a shorter life than the project life, or when excessive wear and tear is expected on equipment such as grinders, dryers, or conveyors.

8.5.3 Land, rent, and local property taxes

Most chemical plants in North America are constructed on rented land or in rented buildings, as it is usually easier and financially more attractive to lease land or property than to tie up capital in purchasing land, putting in the necessary infrastructure, and constructing buildings. Many new plants are built on so-called "*brownfield*" sites that were previously occupied by other process operations. Local governments often provide incentives for companies to redevelop abandoned industrial sites, and chemical companies themselves often encourage other companies to locate plants on unoccupied parts of their site so as to defray some of their own utility and infrastructure costs.

The costs of land or building rental vary widely between locations and play a strong role in determining plant location; see Chapter 11. As a first approximation, the annual rental cost of land is typically taken as 1% of the ISBL plus OSBL capital cost for a plant that has few buildings, or 2% of ISBL plus OSBL capital cost if the plant is to be located indoors.

Some local, regional, state, or provincial governments charge property taxes on commercial land or buildings. The level of property tax should be determined in consultation with local authorities. For a preliminary analysis, 1% of ISBL plus OSBL capital cost can be assumed.

If the land for the plant is purchased, then the cost of land is included in the initial capital cost and no land charge is added to the fixed costs. When land is capitalized, it cannot be depreciated, but the cost of the land is recovered at the end of the project, less any site clean-up and remediation costs.

8.5.4 Insurance

All plants require insurance to cover third-party liability as well as potential plant damage. Most chemical companies maintain insurance coverage through insurance brokers, although some choose to self-insure, essentially setting aside a part of their operating income to cover liabilities. Insurance premiums are based on prior performance and risk assessments carried out by specialist risk management companies and are typically about 1% of ISBL plus OSBL capital cost per year.

8.5.5 Interest payments

If the project is financed by bonds or loans, the regular payments of interest (or interest plus amortization of principal) are a fixed cost of the project. Debt financing is discussed in more detail in Section 9.3.2. Creditors have a primary claim on earnings over shareholders, so payments on debt must be made as a cost of production rather than set aside to be paid out of retained earnings.

Most companies do not break out the relative proportion of debt and equity financing on a project-by-project basis and instead evaluate projects using an overall average cost of capital; see Section 9.3.4. Repayment of debts associated with the fixed capital investment is therefore included with the overall expected return on capital of the project. In this case the FCOP does not include an interest charge associated with the fixed capital investment. It is, however, common to assume that working capital will be funded by entirely by debt, as the value of the working capital is always sufficient to repay the principal of the loan, and the cost of maintaining the working capital is then equal to just the annual interest due. The annual interest payment is then equal to the working capital multiplied by the interest rate, which can be estimated from the interest rate paid on corporate bonds by similar companies; see Section 9.3.2.

When a company has only one plant—for example, when a new venture is being considered—it is best to separate debt financing from equity financing and calculate the cost of servicing the debt as a fixed cost of production. This gives a truer picture of the likely return on equity from the project.

8.5.6 Corporate overhead charges

There are three main contributions to corporate overhead charges:

Research and development costs: R&D costs cover the costs of fundamental discovery projects, new product development, scale-up and testing, clinical trials for new medicines, and applications testing to develop new markets for existing products. R&D costs range from less than 1% of revenues for operating companies in the fuels and bulk petrochemicals sectors to as much as 15% of revenues for some biotechnology and pharmaceuticals companies.

Selling and marketing costs: Selling costs include the costs of paying the sales force, advertising costs including promotional materials, travel to visit customers and trade shows, and other costs associated with closing sales. Additional marketing expenses include the costs of market research and analysis, competitive studies, branding and any other costs associated with developing an understanding of customer needs and preferences, and using this understanding to guide new product development and product positioning and pricing. Selling and marketing costs are highly dependent on the type of product. Bulk commodities that are produced to ASTM standards have almost zero selling and marketing costs, whereas consumer and specialty products can have selling costs as high as 5% of total cost of production.

General and administrative costs: G&A costs include all the costs of administering a corporation: general management; human resources; purchasing and procurement; finance; accounting; strategic planning; business development; property management; information technology; health, safety, and environment; corporate communications; and legal services. In smaller companies some of these functions may be outsourced to consultants, but the costs must nonetheless be borne by the company, and a share of these costs is attributed to any new project. G&A costs can be assessed by looking at the annual income statement of a company (see Section 9.3.1) and give an indication of how bloated the corporate bureaucracy has become. G&A costs are usually

allocated based on either revenue or headcount. A typical initial estimate using a headcount-based approach might be 65% of labor cost plus supervision and overhead, whereas a revenue-based approach would assume the same proportion of revenues as in the overall corporate income statement.

Corporate overhead varies widely depending on the industry sector. Oil refining companies that carry out minimal R&D have much lower overhead than pharmaceuticals manufacturers. Company financial reports can be used to gain insight into the typical distribution of overhead costs in different companies and industries. These reports are freely available and easily obtained over the Internet; see Section 9.3.1.

8.5.7 License fees and royalties

A plant that makes use of proprietary technology must make license or royalty payments to the owner of the technology. If a company practices a technology that is under patent protection without obtaining a license to use the technology, the patent holder can sue them for infringement. If the court finds in favor of the patent holder, then the company can be ordered to cease use of the technology and pay damages.

In the process industries, patents typically cover processes, compositions of matter, chemical and biological routes, process conditions, catalysts, enzymes, genetically modified organisms, processing equipment, and control strategies and algorithms. Patent holders often include royalty fees in the pricing of a product such as a catalyst, enzyme, or piece of equipment, and warrant the customer that their product does not infringe on anyone else's patent.

When the royalty is not included in the price of a product, license fees are negotiated between the patent holder (the licensor) and the company that wants to practice the technology (the licensee). The pricing of the royalty payment depends on the availability of alternatives, the licensee's desire to acquire the technology, and the patent holder's desire to sell. See Section 8.3.1 for a general discussion of pricing. Royalties can be set as a percentage of revenues, but the most common method is a fixed rate per lb or kg of product based on total production capacity. Although the royalty rate is proportional to plant capacity, royalties are a fixed cost and must usually be paid regardless of whether or not the plant actually operates at full capacity.

In some cases, the technology owner will agree to let the licensee capitalize the royalty payments. In this case the licensee pays an up-front amount equal to the sum or net present value of future royalty payments, or some fraction thereof. This arrangement allows the patent holder to recognize revenue sooner and allows the licensee to write off the royalty payments as an initial cost of obtaining the technology rather than a running fixed cost. Both parties are then absolved from the inconvenience of handling regular royalty payments.

8.6 Summarizing revenues and production costs

It is useful to create a single-page summary of all of the production costs and revenues associated with a project, as this makes it easier to review the project economics and understand the relative contribution of different components to the overall cost of production. The summary sheet usually lists the quantity per year and per unit production of product; the price; the cost per year; and the cost per unit production of product for each of the raw materials, by-products, consumables, and utilities, as well as fixed costs and capital charges.

Most chemical companies have a preferred format for summarizing costs of production and often use standard spreadsheets. Good examples are given in the PERP reports published by Nexant (www.nexant.com/products). A template for summarizing production costs is given in Appendix G and can be downloaded in Microsoft Excel format from the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793. The use of this template is illustrated in Example 8.2.

Example 8.2

Adipic acid is used in the manufacture of nylon 6,6. It is made by hydrogenation of phenol to a mixture of cyclohexanol and cyclohexanone (known as KA oil: ketone and alcohol), followed by oxidation with nitric acid. The overall reaction can be written approximately as:

$$C_6H_5OH + 2H_2 \rightarrow C_6H_{10}O$$
$$C_6H_{10}O + H_2 \rightarrow C_6H_{11}OH$$
$$C_6H_{11}OH + 2HNO_3 \rightarrow HOOC(CH_2)_4COOH + N_2O + 2H_2O$$

The actual process requirements of phenol, hydrogen, nitric acid, and utilities and consumables have been determined to be:

Material	Amount	Units
Phenol	0.71572	lb/lb product
Hydrogen	0.0351	lb/lb product
Nitric acid (100% basis)	0.71778	lb/lb product
By-product off-gas	0.00417	lb/lb product
Various catalysts and chemicals	32.85	$/metric ton product
Electric power	0.0939	kWh/lb product
Cooling water	56.1	gal/lb product
HP steam	0.35	lb/lb product
MP steam	7.63	lb/lb product
Boiler feed water	0.04	gal/lb product

These yields were taken from Chem Systems PERP report 98/99-3 Adipic acid (Chem Systems, 1999). The nitric acid consumption is given on a 100% basis, but 60% nitric acid is used in the process.

Estimate the cash cost of production and total cost of production for a new 400,000 metric ton per year (400 kMTA) adipic acid plant located in northeast Asia (the same scale plant introduced in Example 7.8). The prices of adipic acid, phenol, hydrogen, and nitric acid have been forecasted for northeast Asia as $1400/MT, $1000/MT, $1100/MT, and $380/MT, respectively. The price of fuel is $6/GJ (roughly $6/MMBtu), and electricity costs $0.05/kWh. Assume a 15% cost of capital and a 10-year project life.

Solution

It is convenient to summarize costs of production in a spreadsheet, as discussed in Section 8.6. The template from Appendix G has been used in this example and is given in Fig. 8.13. In addition to entering the information from the problem statement into the spreadsheet (with any necessary conversion of units), a few more calculations are needed, as described next.

Closing mass balance

The first thing that is apparent when entering the yield data is that the mass balance for the process does not close properly with the information given. This suggests that we still need to account for some waste streams.

The first waste stream is apparent from the process stoichiometry. Nitric acid is recycled in the process until it is eventually converted to N_2O and vented to the atmosphere. The yield of N_2O can therefore be found by a mass balance on nitrogen:

$$\text{Nitrogen fed} = \text{nitrogen purged}$$

$$400{,}000 \times 0.71778 \times \frac{14}{63} = m_{N20} \times \frac{2 \times 14}{44}$$

Company Name
Address

COST OF PRODUCTION
Adipic Acid from Phenol

Form:XXXXX-YY.ZZ

Project Name	Adipic acid from phenol						
Project Number						Sheet	1
REV	DATE	BY	APVD	REV	DATE	BY	APVD
1	1.1.97	GPT					
2	5.6.20	GPT					

Owner's Name
Plant Location: Northeast Asia
Case Description

Capital Cost Basis Year: 2006 updated to 2020
Units: Metric
On Stream: 8,000 hr/yr; 333.33 day/yr

YIELD ESTIMATE

Yield information taken from ChemSystems PERP report 98/99-3, Adipic Acid, p. 89
Yields input for phenol, nitric acid, hydrogen, off-gas, utilities and consumables

Scale of production set to 400 t/y = 880 MMlb/yr

CAPITAL COSTS

	$MM
ISBL Capital Cost	247.9
OSBL Capital Cost	99.2
Engineering Costs	34.7
Contingency	52.1
Total Fixed Capital Cost	433.9
Working Capital	60.9

REVENUES AND RAW MATERIAL COSTS

MASS BALANCE — MB closure: 101%

Key Products	Units	Units/Unit product	Units/yr	Price $/unit	$MM/yr	$/unit main product
Adipic acid	t	1	400,000	1400	560.00	1400.00
Total Key Product Revenues (REV)	t	1	400,000		560.00	1400.00
By-products & Waste Streams						
Nitrous oxide (vented)	t		100,261	0	0.00	0.00
Off-gas	t	0.00417	1,670	700	1.17	2.92
Organic Waste (Fuel value)	t	0.03072	12,288	300	3.69	9.22
Aqueous Waste	t		273,440	-1.5	-0.41	-1.03
Total Byproducts and Wastes (BP)	t	0.0348939	387,659		4.44	11.11
Raw Materials						
Phenol	t	0.71572	286,288	1000	286.29	715.72
Nitric acid 60% (100% basis)	t	0.71778	287,112	380	109.10	272.76
water with nitric acid	t		191,408	0	0.00	0.00
Hydrogen, 99%	t	0.0351	14,040	1100	15.44	38.61
Total Raw Materials (RM)		1	778,848		410.83	1027.09
			Gross Margin (GM = REV + BP - RM)		153.61	384.03

CONSUMABLES

	Units	Units/Unit product	Units/yr	Price $/unit	$MM/yr	$/unit product
Various catalyst and chemicals	kg	32.85	13,138,263	1.00	13.14	32.85
Other	kg	0	0	0.00	0.00	0.00
Total Consumables (CONS)					13.14	32.85

UTILITIES

	Units	Units/Unit product	Units/hr	Price $/unit	$MM/yr	$/unit product
Electric	kWh	206.0	10,300	0.05	4.120	10.30
HP Steam	t	0.4	18	14.30	2.002	5.01
MP Steam	t	7.6	382	12.00	36.624	91.56
LP Steam	t	0.0	0	8.90	0.000	0.00
Boiler Feed	t	0.3	17	1.10	0.145	0.36
Condensate	t	0.0	0	0.80	0.000	0.00
Cooling Water	t	463.0	23,150	0.024	4.445	11.11
Fuel Fired	GJ	0.0	0	6.00	0.000	0.00
Total Utilities (UTS)					47.336	118.340
			Variable Cost of Production (VCOP = RM - BP + CONS + UTS)		466.86	1167.16

FIXED OPERATING COSTS

			$MM/yr	$/unit product
Labor	4.8	Operators per Shift Position		
Number of shift positions	9	30,000 $/yr each	1.30	3.24
Supervision		25% of Operating Labor	0.32	0.81
Direct Ovhd		45% of Labor & Superv.	0.73	1.82
Maintenance		3% of Fixed Investment	13.02	32.54
Overhead Expense				
Plant Overhead		65% of Labor & Maint.	9.99	24.97
Tax & Insurance		2% of Fixed Investment	6.51	16.27
Interest on Debt Financing		0% of Fixed Capital	0.00	0.00
		6% of Working Capital	3.66	9.14
		Fixed Cost of Production (FCOP)	35.52	88.80

ANNUALIZED CAPITAL CHARGES

	$MM	Interest Rate	Life (yr)	ACCR	$MM/yr	$/unit product
Fixed Capital Investment	433.910	15%	10	0.199	86.46	216.14
Royalty Amortization	15.000	15%	10	0.199	2.99	7.47
Inventory Amortization						
Catalyst 1	0.000	15%	3	0.438	0.00	0.00
Catalyst 2	0.000	15%	3	0.438	0.00	0.00
Adsorbent 1	0.000	15%	3	0.438	0.00	0.00
Equipment 1	0.000	15%	5	0.298	0.00	0.00
Equipment 2	0.000	15%	5	0.298	0.00	0.00
			Total Annual Capital Charge		89.45	223.62

SUMMARY

	$MM/yr	$/unit product
Variable Cost of Production	466.86	1167.16
Fixed Cost of Production	35.52	88.80
Cash Cost of Production	502.38	1255.96
Gross Profit	57.62	144.04
Total Cost of Production	591.83	1479.57

FIG. 8.13 Cost of production worksheet for Example 8.2.

where m_{N2O} is the flow rate of N_2O, which can be calculated as 100,261 MT/y. As a first approximation, there is no cost for handling this stream, although we might revisit this at a more detailed design stage if we need to fit vent scrubbers or other equipment to handle this off-gas.

The second waste stream is also apparent from the overall stoichiometry. Phenol has a molecular weight of 100, and adipic acid has a molecular weight of 146, so the stoichiometric requirement of phenol is = 100/146 = 0.68493 lb/lb product. The actual process consumption has been estimated as 0.71572 lb/lb product, so the difference (0.71572 − 0.68493 = 0.03079 lb/lb) must be converted into organic by-products. It is possible that some of the organic by-product may be material that is lost with the hydrogen-rich fuel gas, but as a first approximation we can assume that we recover an organic liquid waste product from the process. It is also possible (in fact quite likely) that some of the material that we are calling organic by-product is actually losses of organics in the nitrous oxide vent stream. Because this stream probably must be scrubbed before discharge, it is fair to assume as a first approximation that any organic material in it would be collected as an organic waste. This assumption should be revisited at a later stage in the design process when better information on process yields is available. The organic waste stream is priced at a typical fuel value of $300/MT, assuming that it can be burned as process fuel.

The third waste stream is an aqueous waste. This consists of the water that is brought in with the nitric acid, the water formed by the reaction stoichiometry, and any other water consumed, for example, in vent scrubbers or process water washes.

The water brought in with the nitric acid is easily found by mass balance, because it is equal to the mass flow rate of nitric acid (100% basis) × 40/60 = 400,000 × 0.71778 × 4/6 = 191,408 MT/y.

The water formed by reaction stoichiometry can be estimated as 1 mole per mole nitric acid consumed (i.e., 18 MT per 63 MT consumed), giving 400,000 × 0.71778 × 18/63 = 82,032 MT/y. Note that we could also have estimated this as 2 moles per mole product, but that would give an overestimate of the water production, as the amount of nitric acid consumed is less than the apparent stoichiometric requirement. This is because the overall reaction given here is only an approximation and does not include the reaction of cyclohexanone.

The water consumed in process washes and scrubbers is harder to estimate, but because no process water consumption was listed under utilities, we can assume as a first approximation that all the process water needs are met by internal recycles. This gives a total wastewater flow of 191,408 + 82,032 = 273,440 MT/y. The wastewater stream is assigned a cost of $1.5/MT (see Section 8.4.4).

When the values for nitrous oxide, organic waste, and aqueous waste are entered in the spreadsheet, the mass balance shows 101 MT of product for every 100 MT of feed. This is not perfectly closed, but is good enough at this stage in the analysis. The error is most likely in the organic or aqueous waste streams and will have little impact on the economic analysis. This should, of course, be revisited when better process yield data and a converged process simulation are available.

Estimating utility costs

The amounts of utilities consumed are easily estimated from the production rate and the information in the problem statement (with conversion to metric units).

The prices of steam at different levels can be taken from Example 3.2, because the costs of electricity and natural gas are the same. The prices of boiler feed water, condensate, and cooling water are estimated as described in Section 3.2.

The utility cost is about 10% of the variable cost of production. This is typical for many commodity chemical processes.

Estimating fixed costs

This is a relatively complex process and essentially contains two plants: phenol hydrogenation and KA oil oxidation. We should therefore assume at least four shift positions for each plant, say nine total. For a northeast Asian basis we expect that the salary cost per shift position will be lower than the typical $50,000 per year that we would assume for a USGC plant. As a first approximation, this is estimated as $30,000/y. The remaining salary and overhead costs are fixed following the assumptions given in Section 8.5.1.

The total fixed capital cost of this plant was estimated in Example 7.8 to be $433.9MM. Interest charges are not included for the fixed capital (because we will calculate an annualized charge based on overall cost of capital later). An interest charge is included for the working capital, as working capital is recovered at the end of the project and so should not be amortized, as discussed in Section 9.7.2.

The total fixed cost of production is calculated to be $36 MM/y, which is low compared with the variable cost of production ($467 MM/y). It is not uncommon for fixed costs to make a relatively minor contribution to the TCOP for a world-scale plant.

Estimating working capital

The working capital is estimated as 7 weeks' cash cost of production minus 2 weeks' feedstock costs plus 1% of the fixed capital investment, as described in Section 9.2.3. Because the CCOP includes the interest payable on the working capital, this sets up a circular reference in the spreadsheet. The spreadsheet options must be adjusted to ensure that the calculation iterates to convergence. The converged result is \$60.9 MM. Note that the value calculated is about 6% less than it would have been had we estimated the working capital as 15% of fixed capital investment.

Estimating annualized capital costs

The fixed capital investment is to be annualized over 10 years at a 15% interest rate. The method for annualization of capital costs is discussed in Section 9.7.2. For this interest rate and recovery period, the annual capital charge ratio is 0.199, so the annual capital charge is $= 0.199 \times 433.9 =$ \$86.46 MM/y, or \$216.14 /MT of product. As a quick check, we can see that this is roughly 16% of the TCOP, which is in the typical range for commodity chemical processes (10% to 20%).

In addition to the fixed capital investment, we should make an allowance for a process royalty. The problem statement did not specify whether the plant was to be built using proprietary technology, but it is reasonable to assume that a royalty will need to be paid. If a \$15 MM royalty is added, this annualizes to a cost of \$3 MM/y, or roughly 0.5% of revenues, which is a reasonable initial estimate. This should be revisited during more detailed design when discussions with technology vendors take place.

Estimating cost of production

The CCOP is the sum of the fixed and variable production costs (Equation 8.3):

$$\text{CCOP} = \text{VCOP} + \text{FCOP} = 466.86 + 36.94 = \underline{\underline{\$503.81 \text{ MM/y}}}$$

The TCOP is the sum of the CCOP and the annual capital charge (Equation 8.6):

$$\text{TCOP} = \text{CCOP} + \text{ACC} = 502.38 + 89.45 = \underline{\underline{\$591.83 \text{ MM/y}}}$$

It is worth noting that the calculated TCOP is greater than the projected annual revenue of \$560 MM/y. This suggests that the project would not earn the expected 15% interest rate. This is explored further in Examples 9.5, 9.7, and 9.9 and in Problem 9.6.

8.7 References

Chem Systems. (1999). Adipic acid: PERP report 98/99-3. Chem Systems, Inc.

8.8 Nomenclature

		Dimensions in \$MLTθ
ACC	Annual capital charge	**\$**
CCOP	Cash cost of production	$\mathbf{\$M^{-1}}$ or $\mathbf{\$T^{-1}}$
FCOP	Fixed cost of production	$\mathbf{\$M^{-1}}$ or $\mathbf{\$T^{-1}}$
P_F	Price of fuel	$\mathbf{\$M^{-1}L^{-2}T^{2}}$
P_{WFV}	Value of waste as fuel	$\mathbf{\$M^{-1}}$
TCOP	Total cost of production	$\mathbf{\$M^{-1}}$ or $\mathbf{\$T^{-1}}$
VCOP	Variable cost of production	$\mathbf{\$M^{-1}}$ or $\mathbf{\$T^{-1}}$
$\Delta H^\circ c$	Heat of combustion	$\mathbf{L^{-2}T^{2}}$

8.9 Problems

8.1. A gas cleaning plant uses a recirculating alkanolamine solvent to remove H_2S and CO_2 from natural gas. The solvent circulation rate has been estimated to be 2.2 gallons per thousand standard cubic feet of natural gas. The solvent is regenerated using low-pressure steam at a rate of 1.3 lb of steam per gallon of solvent. The solvent is pumped from the regenerator pressure of 1.5 bar gauge to the absorber pressure of 60 bar gauge. The annual cost of solvent make-up for a 50 million scf/d plant is $125,000. If fuel gas costs $6/MMBtu and electricity costs $0.05/kWh, estimate the variable cost per scf of natural gas.

8.2. The consumption of feed and utilities for a plant that produces 60 metric tons per year (60 t/y) of nylon 6 are given here. The plant fixed capital cost has been estimated to be $114 MM. Estimate the cash cost of production.

Raw materials
1. Caprolactam, 1.02 tons per ton product, price $1700 per metric ton
Utilities
1. Fuel gas, 9 MMBtu/t product, cost $4.50/MMBtu
2. Cooling water, 32,000 gal/t product
3. Electrical power, 130 kWh/t product

8.3. The production of methyl ethyl ketone (MEK) is described in Appendix F, Problem F.3. A preliminary design has been made for a plant to produce 10,000 metric tons per year. The plant operating rate will be 8000 hours per year. Estimate the cash cost of production. (Note: The capital cost for this process is estimated in Problem 7.10)

Raw materials
1. 2-butanol, 1.045 kg per kg of MEK, price $800 per metric ton
2. Solvent (trichloroethane) make-up 7000 kg per year, price $1.0/kg
Utilities
3. Fuel oil, 3000 metric tons per year, heating value 45 GJ/metric ton
4. Cooling water, 120 metric tons per hour
5. Steam, low pressure, 1.2 metric tons per hour
6. Electrical power, 1 MW

The fuel oil is burnt to provide flue gases for heating the reactor feed and the reactor. Some of the fuel requirements could be provided by using the by-product hydrogen. Also, the exhaust flue gases could be used to generate steam. The economics of these possibilities need not be considered.

8.4. Natural gas is widely used as fuel in the process industries, so the price of natural gas is often an important variable in economic analysis. Develop a 15-year forecast of U.S. natural gas prices. Historic natural gas prices are available at www.eia.doe.gov. The "industrial" price data set is most typical of the contract prices paid by large industrial consumers. Consider any structural changes that may have occurred in the natural gas market when making your forecast.

8.5. Estimate the price ($/metric ton) in 2010, 2020, and 2030 of:
a. Sulfuric acid, 98 wt%
b. Sodium hydroxide
c. Activated carbon adsorbent
d. Deionized water

8.6. Table 8.3 contains 6-month average price data for styrene and its feedstocks ethylene and benzene for South Korea over the period Jan. 1999 to Dec. 2010. Calculate the gross margin for making styrene from benzene and ethylene, and plot how the gross margin varied over this time period. Develop a forecast of the gross margin of styrene from benzene and ethylene for the time period 2010−2030.

8.7. Use the data in Table 8.3 to construct forecasts of the prices of benzene, ethylene, and styrene in South Korea from 2010 to 2030.

TABLE 8.3 South Korean prices for benzene, ethylene, and styrene (all prices in $/metric ton)

Period	Benzene	Ethylene	Styrene
1H99	218.98	355.67	403.02
2H99	262.86	481.00	603.81
1H00	366.38	520.67	838.58
2H00	404.54	587.83	684.75
1H01	338.19	534.50	529.21
2H01	216.70	467.50	416.08
1H02	293.30	450.67	570.92
2H02	375.11	516.50	659.23
1H03	483.86	580.00	677.75
2H03	415.99	558.17	709.96
1H04	638.07	669.17	870.61
2H04	1055.59	778.83	1278.42
1H05	925.58	829.67	1087.93
2H05	785.97	950.00	1021.90
1H06	815.33	1025.83	1075.45
2H06	931.42	1080.00	1252.43
1H07	1037.46	1122.83	1288.28
2H07	1018.83	1286.83	1341.37
1H08	1145.30	1560.83	1451.25
2H08	846.33	1435.17	1094.41
1H09	539.82	754.83	838.95
2H09	845.93	1096.83	1077.45
1H10	949.62	1252.17	1226.10
2H10	907.75	1221.07	1176.12

Notes:
1. 1H03 denotes the first half of 2003, 2H99 the second half of 1999, etc.
2. Source: CMAI, *www.CMAIglobal.com*.

CHAPTER

9

Economic evaluation of projects

KEY LEARNING OBJECTIVES

- How corporations finance projects
- How to allow for taxes, depreciation, and other investment incentives
- Different criteria that companies use to compare the financial attractiveness of alternative projects and other factors that are also considered in project selection
- How to allow for error in cost estimates
- How to carry out an economic sensitivity analysis

9.1 Introduction

As the purpose of investing money in a chemical plant is to earn more money, some means of comparing the economic performance of projects is needed. Before a company agrees to spend a large amount of capital on a proposed project, the management must be convinced that the project will provide a sound investment compared with other alternatives. This section introduces the principal methods used for making economic comparisons between projects.

9.2 Cash flows during a project

9.2.1 Cash flow diagrams

During any project, cash initially flows out of the company to pay for the costs of engineering, equipment procurement, plant construction, and plant start-up. Once the plant is constructed and begins operation, revenues from the sale of product begin to flow into the company. The estimation of project capital costs is discussed in Chapter 7 and the estimation of revenues and costs of production is described in Chapter 8.

The "net cash flow" at any time is the difference between the earnings and expenditure. A cash flow diagram, such as that shown in Fig. 9.1, shows the forecast cumulative net cash flow over the life of a project. The cash flows are based on the best estimates of investment, operating costs, sales volume, and sales price that can be made for the project. A cash flow diagram gives a clear picture of the resources required for a project and the timing of the earnings. The diagram can be divided into the following characteristic regions:

A–B The investment required to design the plant.
B–C The heavy flow of capital to build the plant and provide funds for start-up, including working capital.

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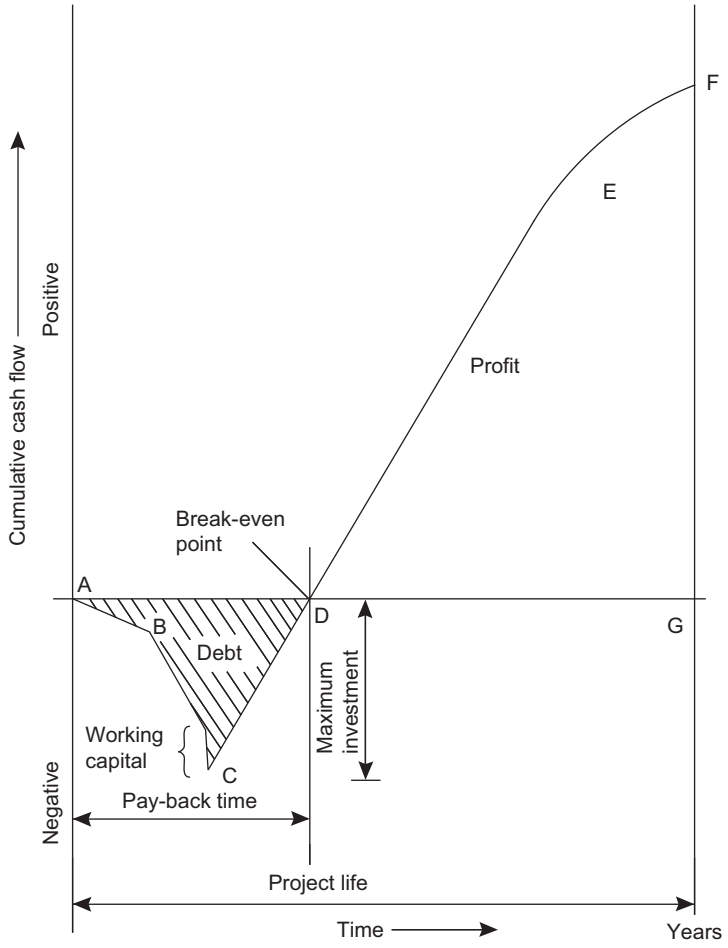


FIG. 9.1 Project cash flow diagram.

C−D The cash flow curve turns up at C, as the process comes on stream and income is generated from sales. The net cash flow is now positive, but the cumulative amount remains negative until the investment is paid off, at point D.
Point D is known as the *break-even point*, and the time to reach the break-even point is called the *pay-back time.* (In a different context, the term "break-even point" is also sometimes used for the percentage of plant capacity at which the income equals the cost of production.)
D−E In this region the cumulative cash flow is positive. The project is earning a return on the investment.
E−F Toward the end of project life the rate of cash flow may tend to fall off because of increased operating costs and falling sales volume and price as a result of obsolescence of the plant, and the slope of the curve changes.
Point F gives the final cumulative net cash flow at the end of the project life.

Net cash flow is a relatively simple and easily understood concept and forms the basis for the calculation of other, more complex, measures of profitability. Taxes and the effect of depreciation are usually not considered in cash flow diagrams.

9.2.2 Cash outflows during design and construction

The rate at which the operating company spends money during the design and construction phase of a project is usually determined by the terms of the contract that they have with an engineering, procurement, and construction (EPC) company. The EPC company, commonly known as a *contractor*, maintains subcontracts with fabricators of pressure vessels, heat exchangers, and other large process equipment, as well as with suppliers of pipe, instruments,

steelwork, wiring, and all the other materials needed to build the plant. The actual purchase (procurement) of individual pieces of equipment is all handled by the contractor.

Most plant construction contracts are divided into several phases based on achievement of defined milestones. A percentage of the total contract amount is payable as each milestone is reached. For example, a common approach is to pay a percentage at signing, at completion of detailed engineering, at groundbreaking, and at mechanical completion and the balance upon successful completion of a performance demonstration run. The exact amount payable at each milestone will be subject to contract negotiations, but the final payment is usually large enough to ensure that contractor will not make any profit until the plant is running properly.

Large projects can take several years to complete. A typical schedule for a single large plant could be a year in detailed engineering and 2 years in construction. Pharmaceutical plants that require regulatory approval can take 5 or 6 years. This is discussed further in Section 9.6.2 (see Table 9.2 for a typical start-up schedule).

9.2.3 Working capital

Working capital is the additional money needed above what it cost to build the plant, start the plant up, and keep the plant running. Working capital is best thought of as the money that is tied up in sustaining plant operation. Working capital typically includes:

1. Value of raw material inventory − usually estimated as 2 weeks' delivered cost of raw materials.
2. Value of product and by-product inventory − estimated as 2 weeks' cost of production.
3. Cash on hand − estimated as 1 week's cost of production.
4. Accounts receivable − products shipped but not yet paid for; estimated as 1 month's cost of production, but could be larger depending on customer payment terms.
5. Credit for accounts payable − feedstocks, solvents, catalysts, packaging, etc., received but not yet paid for; estimated as 1 month's delivered cost, but could be larger depending on terms negotiated with vendors.
6. Spare parts inventory − estimated as 1% to 2% of inside battery limits (ISBL) plus outside battery limits (OSBL) investment cost.

It can be seen that the sum of items 1 through 5 is roughly 7 weeks' cost of production minus 2 weeks' feedstock costs (item 5 is a credit).

Working capital can vary from as low as 5% of the fixed capital for a simple, single-product process, with little or no finished product storage, to as high as 30% for a process producing a diverse range of product grades for a sophisticated market, such as synthetic fibers. A typical figure for petrochemical plants is 15% of the fixed capital (ISBL plus OSBL cost).

Working capital is better estimated from the cost of production rather than the capital investment. The rules of thumb given earlier can be used to make a preliminary estimate of the working capital required.

Working capital is still required as long as the plant is in operation, and it should not be confused with miscellaneous start-up costs. The working capital that is tied up in operating the plant can be reduced by tighter management of inventories and accounts receivable, and these are the goals of lean management methods. Working capital is recovered at the end of the plant life when the remaining inventories are eliminated. Working capital cannot be depreciated because it does not lose value due to "wear and tear."

Companies will sometimes discuss working capital turns, or turnover, defined as the ratio of annual revenues divided by average working capital. Working capital turnover can be increased by reducing working capital. Higher (or increasing) values of working capital turns indicate that the leaders of a business are managing working capital efficiently.

Other methods for estimating the working capital requirement are given by Bechtel (1960), Lyda (1972), and Scott (1978).

9.2.4 Cash flows at the end of the project

If a plant ceases operation, or is "mothballed" (shut down on a semi-permanent basis), then the working capital is recovered, but must be reinvested if the plant is restarted. When a plant is shut down permanently, it can be sold in its entirety or else broken up and sold as scrap. Several companies specialize in buying and reselling secondhand plants, and advertisements for used plants and equipment can usually be found in the classified sections of the trade journals and on resale websites such as www.equipnet.com. The scrap value can be estimated based on the

equipment weight and is usually less than 10% of the ISBL investment. OSBL investments are not recovered unless the entire site is shut down.

If land was purchased for the plant, which is increasingly uncommon, then the land can be sold as an additional end-of-life credit. Site remediation costs must be subtracted from the value of the land, so the additional cash flow from the sale of land is not necessarily positive.

These cash flows at the end of the project are often not included in profitability analysis, as their timing is uncertain and they are often far enough in the future that they have negligible impact on any of the measures of profitability.

9.3 Project financing

The construction and operation of chemical plants require large amounts of capital. Corporations engaged in the production of chemicals must raise the finances to support such investments. Like taxation, corporate financing is a specialized subject with many intricacies that require expert knowledge. The way a corporation raises funds to finance projects determines the cost of capital for that corporation, and hence sets the expected financial rate of return that the projects must achieve. The design engineer therefore needs a superficial awareness of this subject to carry out economic analysis and optimization of the design.

9.3.1 Basics of corporate accounting and finance

The purpose of financial accounting is to report the economic performance and financial condition of a company to its owners (shareholders), lenders, regulatory agencies, and other stakeholders. The primary means for financial reporting is the annual report to shareholders. The annual reports for companies in the chemical, pharmaceutical, and fuels industries generally contain:

1. A letter from the chief executive officer (CEO) describing the past year's operations, significant acquisitions, divestitures and restructuring, and plans for the short and long term
2. Financial information:
   - **a.** Balance sheet
   - **b.** Income statement
   - **c.** Cash flow statement
   - **d.** Notes to the financial statements
   - **e.** Comments from the independent auditors
3. Information on the directors and executive management of the company
4. A report on the health, safety, and environmental performance of the company (sometimes published separately)

The annual report of any publicly traded company will usually be available online and can easily be found by visiting the company's website. The site will usually have a prominent link to "information for investors" or something similar. No attempt has been made to create fictitious financial statements for the purposes of this book, as an abundance of real examples is readily available online. The reader is encouraged to search online for real cases to study.

Balance sheet

The balance sheet is a snapshot of the financial condition of the company. It lists all the assets owned by the company and all the liabilities or amounts owed by the company. The difference between assets and liabilities is the stockholder's equity (i.e., notionally the amount of money the stockholders would have available to share out if they decided to liquidate the company).

$$\text{Stockholder's equity} = \text{assets} - \text{liabilities} \tag{9.1}$$

Assets are traditionally listed in order of decreasing liquidity. Liquidity is a measure of how easily the asset could be turned into cash. Assets include:

- Cash and cash equivalents.
- Notes and accounts receivable (i.e., money owed to the company for goods shipped but not yet paid for).
- Inventories of raw materials, products, spare parts, and other supplies.

- Prepaid taxes and expenses.
- Investments such as equity stakes in other companies or joint ventures.
- Property, plant, and equipment. This is listed at book value (i.e., cost less accumulated depreciation). The actual market value of these assets may be considerably higher.
- Intangible assets such as patents, trademarks, goodwill, etc.

Liabilities are usually listed in the order in which they are due, starting with current liabilities. Liabilities include:

- Accounts payable (i.e., payment owed on goods already received by the company).
- Notes and loans due for repayment.
- Accrued liabilities and expenses such as legal settlements, amounts set aside for warranties, guarantees, etc.
- Deferred income taxes.
- Long-term debt.

The difference between assets and liabilities is the shareholder's equity. This consists of the capital paid in by the owners of common and preferred stocks, together with earnings retained and reinvested in the business. The capital paid in by the shareholders is often listed as the par value of the stock (typically 25¢ to $1 per share) plus the additional capital paid in when the stock was initially sold by the company. Note that this reflects only the capital raised by the company and has no relation to subsequent increases or decreases in the value of the stock that may have resulted from trading on the stock market.

Income statement

The income statement or consolidated statement of operations is a summary of the incomes, expenditures, and taxes paid by the company over a fixed period. Results are usually presented for the past 3 calendar years.

The income statement lists the following items:

1. Sales and operating revenues (positive)
2. Income from equity holdings in other companies (positive)
3. Cost of goods sold (negative)
4. Selling, general, and administrative expenses (negative)
5. Depreciation (negative on the income statement, but will be added back on the cash flow statement)
6. Interest paid on debt (negative)
7. Taxes other than income tax, such as excise duties (negative)
8. Income taxes (negative)

The sum of items 1 through 5 is sometimes listed as earnings before interest and taxes (EBIT). The sum of items 1 through 7 is listed as income before taxes, or taxable income, and is usually positive. The net income is the sum of items 1 through 8 (i.e., income before taxes minus taxes paid). Net income is also usually expressed as earnings per share of common stock.

The fixed and variable costs discussed in Chapter 8 generally fall into the category of cost of goods sold, except that the costs of corporate functions such as research and development, marketing, finance, information technology, legal, and human resources are usually rolled up into the selling, general, and administrative (SG&A) expenses.

The income statement gives a good insight into the overall profitability and margins of a business. It has to be read carefully, though, as several items listed are noncash charges, such as depreciation, that do not affect the cash flow of the business. Corrections for these items are made in the cash flow statement.

Cash flow statement

The cash flow statement gives a summary of overall cash flows into and out of the business as a result of operating activities, investments, and financing activities. It is also usually reported for the past 3 calendar years.

The cash flow from operating activities section starts with the net income. Adjustments are made for noncash transactions (depreciation and deferred taxes are added back in) and changes in assets and liabilities.

The cash flow from investing activities section lists the cash spent on acquiring fixed assets such as property, plant, and equipment, less any revenues from the sale of fixed assets. It also lists acquisitions or divestitures of subsidiary businesses.

The cash flow from financing activities section summarizes changes in the company's long-term and short-term debt, proceeds from issues of common stock, repurchase of stocks, and dividends paid to stockholders.

The sum of cash flows from operations, investments, and financing gives the net change in cash and cash equivalents. This is then added to the cash and cash equivalents from the beginning of the year to give the cash and cash equivalents at the end of the year, which appears on the balance sheet.

Summary

The business and accounting literature contains a wealth of information on how to read and analyze corporate financial statements. Most engineers work for or with corporations and have a direct personal interest in understanding financial performance; however, a detailed treatment of the subject is beyond the scope of this book. Excellent introductions to finance and accounting are given in the books by Spiro (1996), Fields (2016), and Shim and Henteleff (1995).

9.3.2 Debt financing and repayment

Most debt capital is raised by issuing long-term bonds. A mortgage is a bond that is backed by pledging a specific real asset as security against the loan. An unsecured bond is called a *debenture*. The ratio of total debt divided by total assets is known as the *debt ratio* (DR), or leverage of the company.

All debt contracts require payment of interest on the loan and repayment of the principal (either at the end of the loan period or amortized over the period of the loan). Interest payments are a fixed cost, and if a company defaults on these payments, its ability to borrow money will be drastically reduced. Because interest is deducted from earnings, the greater the leverage of the company, the higher the risk to future earnings, and hence to future cash flows and the financial solvency of the company. In the worst case, the company could be declared bankrupt and the assets of the company sold off to repay the debt. Finance managers therefore carefully adjust the amount of debt owed by the company so that the cost of servicing the debt (the interest payments) does not place an excessive burden on the company.

The rate of interest owed on debt depends on the bond markets, government central banks, and the credit worthiness of the company. When new bonds are issued, they must be offered at a competitive interest rate; otherwise, they will not sell. If the bond issuer has a high credit rating, they will be able to issue bonds at low interest rates, close to the interest rates set by the government for government bonds. (Most governments try to maintain a high credit rating and avoid defaulting on their bonds so that they can continue to borrow money at low interest rates.) If the credit rating of the issuer is lower, there is a higher chance that the debt may not be repaid, in which case it must be offered at a higher interest rate to offset this risk. Credit rating services such as Moody's and Standard & Poor's study the finances of governments and corporations and publish credit ratings. These ratings are usually not advertised by issuers unless they are very high, but they are published in the financial papers. The difference in interest rate between low-rated and high-rated bonds issued at the same time is typically 2% to 3%.

Once they have been issued, bonds are traded on the New York Stock Exchange, the American Stock Exchange, or other global financial exchanges. Although the price of the bond in subsequent trading may vary from the offer price (or face value), the interest rate remains fixed. The *Wall Street Journal* reports prices daily for the most actively traded corporate bonds. Bond prices can also be found at the Financial Industry Regulatory Authority (FINRA) website (http://finra-markets.morningstar.com/MarketData/), together with a lot of other useful information on bond markets and investing The interest rate is listed as the "coupon," and the date on which the bond expires is the "maturity." Bonds are also assigned a unique nine-digit identification number by the American Bankers' Association Committee on Uniform Security Identification Procedures (CUSIP). For example, in 2006 Honeywell, Inc., issued a 30-year bond CUSIP #438516AR7 with coupon 5.700 and maturity 03/15/2036.

9.3.3 Equity financing

Equity capital consists of the capital contributed by stockholders, together with earnings retained for reinvestment in the business. Stockholders purchase stocks in the expectation of getting a return on their investment. This return can come from the dividends paid annually to stockholders (the part of earnings returned to the owners) or from growth of the company that is recognized by the stock market and leads to an increase in the price of the stock.

Most stock is usually held by sophisticated institutional investors such as banks, mutual funds, insurance companies, and pension funds. These investors employ expert analysts to assess the performance of companies relative to other companies in the same sector and to the market as a whole. If the management of a company

does not deliver the financial return expected by investors, the stock price will suffer and the management will soon be replaced.

Simple measures of the effectiveness of management are the return on equity (ROE) and earnings per share. ROE is defined as:

$$\text{ROE} = \frac{\text{net annual profit}}{\text{stockholders' equity}} \times 100\% \tag{9.2}$$

The stockholders' expectation of return on their equity can be expressed as an interest rate and is known as the *cost of equity capital*. The cost of equity required to meet the expectations of the market is usually substantially higher than the interest rate owed on debt because of the riskier nature of equity finance (because debt holders are paid first and hence have the primary right to any profit made by the business). For most corporations in the United States at the time of writing, the cost of equity is in the range 25% to 30%.

9.3.4 Cost of capital

Very few companies operate entirely on debt or equity financing alone, and most use a balance of both. The overall cost of capital is simply the weighted average of the cost of debt and the cost of equity.

$$i_c = (DR \times i_d) + ((1 - DR) \times i_e) \tag{9.3}$$

where: i_c = cost of capital
DR = debt ratio
i_d = interest rate due on debt
i_e = cost of equity

For example, if a company were financed 55% with debt at an average 8% interest and 45% with equity that carried an expectation of a 25% return, then the overall cost of capital would be:

$$i_c = (0.55 \times 0.08) + (0.45 \times 0.25)$$

$$\underline{\underline{= 0.1565}}$$

Because the equity is by definition (Equation 9.1) the assets minus the liabilities (debt), the overall return on assets (ROA) can be expressed as:

$$\text{ROA} = \frac{\text{net annual profit}}{\text{total assets}} \times 100\% \tag{9.4}$$

It follows that:

$$\frac{\text{ROA}}{\text{ROE}} = \frac{\text{stockholders' equity}}{\text{total assets}} = 1 - DR \tag{9.5}$$

The overall cost of capital sets the interest rate that is used in economic evaluation of projects. The total portfolio of projects funded by a company must meet or exceed this interest rate if the company is to achieve its targeted ROE and hence satisfy the expectations of its owners.

9.4 Taxes and depreciation

The profits generated by most chemical plants are subject to taxation. Taxes can have a significant impact on the cash flows from a project. The design engineer needs to have a basic understanding of taxation and tax allowances such as depreciation to make an economic evaluation of the project.

9.4.1 Taxes

Individuals and corporations must pay income tax in most countries. The details of tax law can be complicated, and governments enact changes almost every year. Companies generally retain tax specialists, either as employees or as consultants, who have deep expertise in the intricacies of the field. Such specialized knowledge is not required

for engineering design projects, which are usually compared on a relatively simple after-tax basis. The design engineer may occasionally need to consult a tax expert, though, particularly when comparing projects in different countries with different tax laws.

Information on corporate taxes in the United States is given on the Internal Revenue Service website at www.irs.gov. At the time of writing, the rate of federal income tax on corporations in the United States is 21% (IRS Publication 542). In many locations corporations must also pay state or local income taxes.

In Canada, corporations pay income tax under the Canadian Income Tax Act (R.S.C., 1985, c. 1 (5th Supp.)). Information on the Canadian Income Tax Act can be obtained from www.laws-lois.justice.gc.ca.

The amount of tax that must be paid in a given year is calculated by multiplying the taxable income by the tax rate. The taxable income is given by:

$$\text{Taxable income} = \text{gross profit} - \text{tax allowances} \tag{9.6}$$

Various types of tax allowances are permitted in the tax laws of different countries, the most common of which is depreciation, discussed in Section 9.4.3. The after-tax cash flow is then:

$$\begin{aligned} CF &= P - (P - D)t_r \\ &= P(1 - \mathrm{t_r}) + Dt_r \end{aligned} \tag{9.7}$$

where: CF = after-tax cash flow
P = gross profit
D = sum of tax allowances
t_r = rate of taxation

It can be seen from Equation 9.7 that the effect of tax allowances is to reduce taxes paid and increase cash flow.

In some countries, taxes are paid in a given year based on the previous year's income. This is true for the United States, where corporate taxes are based on a calendar year of operations and are due by March 15 of the following year. This complicates the calculations somewhat, but is easily coded into a spreadsheet.

9.4.2 Investment incentives

National and regional governments often provide incentives to encourage companies to make capital investments, because these investments create employment, generate taxation revenue, and provide other benefits to politicians and the communities they represent.

The most common incentives used are tax allowances. Most countries allow some form of depreciation charge as a tax allowance, by which the fixed capital investment can be deducted from taxable income over a period, as described in Section 9.4.3. Other incentives that are often used include:

1. Tax waivers or vacations, in which no taxes are paid for a fixed period, typically 2 to 5 years after the project begins generating revenue.
2. Investment grants or credits, in which the government makes a cash contribution towards the initial investment.
3. Low-cost loans, in which the government either loans capital directly or else subsidizes the interest due on a commercial loan.
4. Loan guarantees, in which the government agrees to underwrite loans for the project, reducing the risk of the loan and hence making it easier to secure financing on advantageous terms.

Any economic comparison between different process alternatives for the same site should usually be made using the same assumptions on investment incentives. This might not always be the case, though, for example, if one project is eligible for a government grant because of using renewable energy and another project is not. It should also be noted that differences in incentives can have a significant impact on investment decisions when comparing investments at a company-wide level in a global context.

9.4.3 Depreciation charges

Depreciation charges are the most common type of tax allowance used by governments as an incentive for investment. Depreciation is a noncash charge reported as an expense, which reduces income for taxation purposes. There is no cash outlay for depreciation, and no money is transferred to any fund or account, so the depreciation charge is added back to the net income after taxes to give the total cash flow from operations.

$$\begin{aligned} CF &= I - (I \times t_r) + D \\ &= (P - D) - ((P - D) \times t_r) + D \\ &= P(1 - t_r) + Dt_r \end{aligned} \tag{9.8}$$

where: I = taxable income
D = depreciation tax allowance

It can be seen that Equations 9.7 and 9.8 are equivalent.

Depreciation charges can be thought of as an allowance for the "wear and tear, deterioration or obsolescence of the property" as a result of its use (IRS publ. 946).

The book value of an asset is the original cost paid minus the accumulated depreciation charged. The book value has no connection to the resale value or current market value of the asset.

$$\text{Book value} = \text{initial cost} - \text{accumulated depreciation} \tag{9.9}$$

Note that the law usually only allows depreciation of fixed capital investments and not total capital, because working capital is not consumed and can be recovered at the end of the project. If land was purchased for the project, then the cost of the land must be deducted from the fixed capital cost, as land is assumed to retain its value and cannot be depreciated.

Over time the book value of the asset or fixed investment decreases until it is fully "paid off" or "written off," at which point depreciation can no longer be charged. The schedule of how depreciation charges are taken is set by the tax law. In the United States, most investments are depreciated using either straight-line depreciation or the Modified Accelerated Cost Recovery System (MACRS) described later (IRS publ. 946), but other methods are used internationally, and in a globalized economy it is necessary for design engineers to have familiarity with these also.

Straight-line depreciation

Straight-line depreciation is the simplest method. The depreciable value, C_d, is depreciated over n years with annual depreciation charge D_i in year i, where:

$$D_i = \frac{C_d}{n} \quad \text{and} \quad D_j = D_i \quad \forall\, j \tag{9.10}$$

The depreciable value of the asset is the initial cost of the fixed capital investment, C, minus the salvage value (if any) at the end of the depreciable life. For chemical plants, the salvage value is often taken as zero, as the plant usually continues to operate for many years beyond the end of the depreciable life.

The book value of the asset after m years of depreciation, B_m is:

$$\begin{aligned} B_m &= C - \sum_{i=1}^{m} D_i \\ &= C - \frac{mC_d}{n} \end{aligned} \tag{9.11}$$

When the book value is equal to the salvage value (or zero), then the asset is fully depreciated and no further depreciation charge can be taken.

Straight-line depreciation must be used in the United States for software (with a 36-month depreciable life), patents (with life equal to the patent term remaining), and other depreciable intangible property (IRS publ. 946).

Straight-line depreciation is allowed under the U.S. tax code for other classes of property, with defined life depending on the type of asset. Although straight-line depreciation is not as favorable as the accelerated methods described in the following sections, it is still the preferred method for most large corporations. This is because it is difficult and costly for an established company to change accounting methods, and most large corporations have used straight-line depreciation in previous years.

Declining-balance depreciation

The declining-balance method is an accelerated depreciation schedule that allows higher charges in the early years of a project. This helps improve project economics by giving higher cash flows in the early years. In the declining-balance method, the annual depreciation charge is a fixed fraction, F_d, of the book value:

$$D_1 = C\,F_d \tag{9.12}$$
$$B_1 = C - D_1 = C(1-F_d)$$
$$D_2 = B_1 F = C(1-F_d)F_d$$
$$B_2 = B_1 - D_2 = C(1-F_d)(1-F_d) = C(1-F_d)^2$$

Hence:

$$D_m = C(1-F_d)^{m-1}F_d \tag{9.13}$$
$$B_m = C(1-F_d)^m \tag{9.14}$$

The fraction F_d must be equal to or less than $2/n$, where n is the depreciable life in years. When $F_d = 2/n$, this method is known as *double declining-balance depreciation.*

Modified Accelerated Cost Recovery System

The MACRS depreciation method was established by the U.S. Tax Reform Act of 1986. The details of the MACRS depreciation method are given in IRS publication 946, which is available online at www.irs.gov/publications. The method is basically a combination of the declining-balance method and the straight-line method. The declining-balance method is used until the depreciation charge becomes less than it would be under the straight-line method, at which point the MACRS method switches to charge the same amount as the straight-line method.

Under MACRS depreciation, different recovery periods are assigned to different kinds of asset, based on a usable life ("class life") designated by the U.S. Internal Revenue Service. For chemicals manufacture, the latest version of the IRS publication 946 at the time of writing lists a class life of 9.5 years and a recovery period of 5 years (see www.irs.gov/publications/P946 Appendix B). Class life for other process industries ranges from 7.5 years for offshore oil production to 18 years for coal gasification, sugar production, and vegetable oil purification. Always consult the IRS publication to determine the appropriate schedule for a given project. It should be noted, however, that for roads, docks, and other civil infrastructure a 15-year recovery period is used, whereas for cogeneration, power transmission, and natural gas piping the recovery period is 20 years, so some offsite investments are depreciated on a different schedule from that used for the ISBL investment.

Another important convention within MACRS depreciation is that the method assumes that all property is acquired mid-year and hence assigns half of the full year's depreciation in the first and last years of the recovery period. The result is the schedule of depreciation charges given in Table 9.1.

There are other details of MACRS depreciation that are not discussed here, and at the time of writing the tax law also allows assets to be depreciated by the straight-line method (over the class life, not the recovery period, and still

TABLE 9.1 MACRS depreciation charges

	Depreciation rate ($F_i = D_i/C_d$)		
Recovery year	**Five-year recovery**	**Seven-year recovery**	**Fifteen-year recovery**
1	20	14.29	5.00
2	32	24.49	9.50
3	19.2	17.49	8.55
4	11.52	12.49	7.70
5	11.52	8.93	6.93
6	5.76	8.92	6.23
7		8.93	5.90
8		4.46	5.90
9			5.91
10			5.90

TABLE 9.1 MACRS depreciation charges—cont'd

	Depreciation rate ($F_i = D_i/C_d$)		
Recovery year	**Five-year recovery**	**Seven-year recovery**	**Fifteen-year recovery**
11			5.91
12			5.90
13			5.91
14			5.90
15			5.91
16			2.95

following the half-year convention). Many large corporations use straight-line depreciation instead of MACRS, as they have historically used the straight-line method and do not want the added costs and financial uncertainty of changing the accounting approach.

The tax law is revised frequently, and the most recent version of IRS publication 946 should be consulted for the current regulations. Similarly, when analyzing international projects, the appropriate national and regional tax laws must be checked to ensure that the correct depreciation rules are followed. There are several other less widely used depreciation methods that are not discussed here. A good overview of these is given by Humphreys (1991).

Example 9.1

A chemical plant with a fixed capital investment of $100 million generates an annual gross profit of $50 million. Calculate the depreciation charge, taxes paid, and after-tax cash flows for the first 10 years of plant operation using straight-line depreciation over 10 years and using MACRS depreciation with a 5-year recovery period. Assume the plant is built at time zero and begins operation at full rate in year 1. Assume the rate of corporate income tax is 21% and taxes must be paid based on the previous year's income.

Solution

The solution is easily coded into a spreadsheet. The results are shown in the following tables:

Solution 9.1a

Year	Gross profit (MM$)	Depreciation charge (MM$)	Taxable income (MM$)	Taxes paid (MM$)	Cash Flow (MM$)
0	0	0	0	0	–100
1	50	10	40	0	50
2	50	10	40	8.4	41.6
3	50	10	40	8.4	41.6
4	50	10	40	8.4	41.6
5	50	10	40	8.4	41.6
6	50	10	40	8.4	41.6
7	50	10	40	8.4	41.6
8	50	10	40	8.4	41.6
9	50	10	40	8.4	41.6
10	50	10	40	8.4	41.6

Solution 9.1b

Year	Gross profit (MM$)	Depreciation charge (MM$)	Taxable income (MM$)	Taxes paid (MM$)	Cash Flow (MM$)
0	0	0	0	0	–100
1	50	20	30	0	50
2	50	32	18	6.30	43.70
3	50	19.2	30.8	3.78	46.22
4	50	11.52	38.48	6.47	43.53
5	50	11.52	38.48	8.08	41.92
6	50	5.76	44.24	8.08	41.92
7	50	0	50	9.29	40.71
8	50	0	50	10.50	39.50
9	50	0	50	10.50	39.50
10	50	0	50	10.50	39.50

9.5 Simple methods for economic analysis

This section introduces some economic measures that can be estimated quickly if the project investment and cash flows are known. These methods are widely used for preliminary "eyeballing" of project attractiveness, and in some companies they are used for preliminary screening of projects. They are not suitable for detailed project selection, as they involve too many simplifying assumptions. The choice of which method to use in a particular application is addressed in Section 9.9.3.

9.5.1 Pay-back time

A simple method for estimating the pay-back time is to divide the total initial capital (fixed capital plus working capital) by the average annual cash flow:

$$\text{simple pay-back time} = \frac{\text{total investment}}{\text{average annual cash flow}} \tag{9.15}$$

This is not the same pay-back time indicated by the cash flow diagram, as it assumes that all the investment is made in year zero and revenues begin immediately. For most chemical plant projects, this is not realistic, as investments are typically spread over 1 to 3 years and revenues may not reach 100% of design basis until the second year of operation. The simple pay-back time is strictly based on a cash flow, but for simplicity, taxes and depreciation are often neglected and the average annual income is used instead of cash flow.

9.5.2 Return on investment

Another simple measure of economic performance is the return on investment (ROI). The ROI is defined in a similar manner to ROA and ROE:

$$\text{ROI} = \frac{\text{net annual profit}}{\text{total investment}} \times 100\% \tag{9.16}$$

Net annual profit is the same as annual operating income after tax. If ROI is calculated as an average over the whole project, then:

$$\text{ROI} = \frac{\text{cumulative net profit}}{\text{plant life} \times \text{initial investment}} \times 100\% \tag{9.17}$$

Calculation of the after-tax ROI is complicated if the depreciation term is less than the plant life and if an accelerated method of depreciation such as MACRS is used. In such cases, it is just as easy to calculate one of the more meaningful economic criteria such as net present value or discounted cash flow rate of return, described later. Because of this complication, a pretax ROI is often used instead:

$$\text{pretax ROI} = \frac{\text{pretax cash flow}}{\text{total investment}} \times 100\% \tag{9.18}$$

Note that pretax ROI is based on cash flow, not profit or taxable income, and therefore does not include a depreciation charge.

ROI is also sometimes calculated for incremental modifications to a large project, as described in Section 9.9.3.

Example 9.2

Calculate the simple pay-back time, ROI, and pretax ROI for the project introduced in Example 9.1, assuming MACRS depreciation is used.

Solution

If we base the simple pay-back on income instead of cash flow, it is:

$$\text{Simple pay-back (before tax)} = \frac{\$\ 100\ \text{MM}}{\$\ 50\ \text{MM/yr}} = \underline{\underline{2\ \text{years}}}$$

If, instead, we average the cash flows after allowing for taxes and depreciation, then using the numbers from the solution to Example 9.1b, we obtain average annual cash flow = $42.65 MM, in which case:

$$\text{Simple pay-back (after tax)} = \frac{\$\ 100\ \text{MM}}{\$\ 42.65\ \text{MM/yr}} = \underline{\underline{2.34\ \text{years}}}$$

The ROI can be calculated from Equation 9.17:

$$\text{ROI} = \frac{426.5}{10 \times 100} \times 100\% = \underline{\underline{42.65\%}} \tag{9.17}$$

The pretax ROI is just the inverse of the before-tax simple pay-back and is 50/100 = 50%.

Note that calculation of the after-tax pay-back time and ROI requires calculation of the schedule of depreciation charges and taxes. Because this usually involves creating a table or spreadsheet, most of the effort required to calculate more useful economic measures has already been invested. Simple pay-back and ROI are therefore often only used on a before-tax basis.

Example 9.3

A plant is producing 10,000 metric tons per year (10 kt/y or 10 kMTA) of a product. The overall yield is 70 wt% (0.7 kg of product per kg raw material). The raw material costs $500/metric ton, and the product sells for $900/metric ton. A process modification has been devised that will increase the yield to 75%. The additional investment required is $1,250,000, and the additional operating costs are negligible. Is the modification worth making?

Solution

There are two ways of looking at the earnings to be gained from the modification:

1. If the additional production given by the yield increase can be sold at the current price, the earnings on each additional ton of production will equal the sales price less the raw material cost.
2. If the additional production cannot be readily sold, the modification results in a reduction in raw material requirements rather than increased sales, and the earnings (savings) are from the reduction in annual raw material costs.

The second way gives the lowest figures and is the safest basis for making the evaluation. At 10 kMTA production:

$$\text{Raw material requirements at 70\% yield} = \frac{10{,}000}{0.7} = 14{,}286$$

$$\text{at 75\% yield} = \frac{10{,}000}{0.75} = 13{,}333$$

$$\text{Cost savings} = 953\ \text{t/y, which is worth } 953 \times 500 = \$476{,}500/\text{y}$$

$$\text{Pretax ROI} = \frac{476{,}500}{1{,}250{,}000} = \underline{\underline{38\%}}$$

As the annual savings are constant, the pretax simple pay-back period is the inverse of the pretax ROI:

$$\text{Simple pay} - \text{back period} = \frac{1{,}250{,}000}{476{,}500} = 2.62\ \text{years}$$

Based on the attractive ROI and pay-back period, this investment would seem to be worth pursuing further. Whether or not it was implemented would depend on the hurdle rate set for investments by the company.

9.6 Present value methods

The simple economic measures introduced in Section 9.5 are not able to capture the time dependence of cash flows during the project. The timing of cash flows is very important to investors, first because not all of the capital must be

financed immediately, and second because capital that is repaid sooner can be put back to work in another investment. Present value methods account for this *time value of money* and are preferred over simple methods when evaluating large investments; see Section 9.9.3.

9.6.1 Time value of money

In Fig. 9.1 the net cash flow is shown at its value in the year in which it occurred. So the figures on the ordinate show the "future worth" of the project. The cumulative value is the "net future worth" (NFW).

The money earned in any year can be reinvested as soon as it is available and can start to earn a return. So money earned in the early years of the project is more valuable than that earned in later years. This "time value of money" can be allowed for by using a variation of the familiar compound interest formula. The net cash flow in each year of the project is brought to its "present value" at the start of the project by discounting it at some chosen compound interest rate.

Future worth

The future worth of an amount of money, P, invested at interest rate, i, for n years is:

$$\text{Future worth in year } n = P(1+i)^n$$

Hence the present value of a future sum is:

$$\text{present value of future sum} = \frac{\text{future worth in year } n}{(1+i)^n} \tag{9.19}$$

The interest rate used in discounting future values is known as the *discount rate* and is chosen to reflect the earning power of money. In most companies the discount rate is set at the cost of capital (see Section 9.3.4).

Inflation

Discounting of future cash flows should not be confused with allowing for price inflation. Inflation is a general increase in prices and costs, usually caused by imbalances between supply and demand. Inflation raises the costs of feed, products, utilities, labor, and parts, but does not affect depreciation charges, which are based on original cost. Discounting, on the other hand, is a means of comparing the value of money that is available now (and can be reinvested) with money that will become available at some time in the future. All of the economic analysis methods can be modified to allow for inflation. See, for example, Humphreys (1991), Chapter 6. In practice, most companies assume that although prices may suffer inflation, margins and hence cash flows will be relatively insensitive to inflation. Inflation can therefore be neglected for the purposes of comparing the economic performance of projects.

9.6.2 Net present value

The net present value (NPV) of a project is the sum of the present values of the future cash flows:

$$\text{NPV} = \sum_{n=1}^{n=t} \frac{CF_n}{(1+i)^n} \tag{9.20}$$

where: CF_n = cash flow in year n
t = project life in years
$\mathbf{i}$= interest rate (= cost of capital, percent /100)

The NPV is always less than the total future worth of the project because of the discounting of future cash flows. NPV is easily calculated using spreadsheets, and most spreadsheet programs have a NPV function.

The NPV is a strong function of the interest rate used and the period studied. When different periods are analyzed, the period is sometimes denoted by a subscript. For example, NPV_{10} would denote the NPV over a 10-year period.

NPV is a more useful economic measure than simple pay-back and ROI, because it allows for the time value of money and for annual variation in expenses and revenues. Few large projects are completed in a single year and immediately begin production at full capacity. A more typical start-up schedule for a chemical process is given in Table 9.2. For pharmaceutical products, the time scale can be even longer, as the plant must be certified to be in compliance with good manufacturing practices (cGMP) and must be inspected and approved by the Food and Drug Administration (FDA) before production can begin. The time from breaking ground to production for new pharmaceutical products produced by fermentation is typically about 6 years (Lee, 2010). NPV is also a more appropriate method to use when considering after-tax income using an accelerated depreciation method such as MACRS.

9.6.3 Discounted cash flow rate of return

By calculating the NPV at various interest rates, it is possible to find an interest rate at which the cumulative NPV at the end of the project is zero. This particular rate is called the *discounted cash flow rate of return* (DCFROR) and is a measure of the maximum interest rate that the project could pay and still break even by the end of the project life.

TABLE 9.2 Typical start-up schedule

Year	Costs	Revenues	Explanation
1st year	30% of fixed capital	0	Engineering + long lead-time items
2nd year	40%–60% of fixed capital	0	Procurement and construction
3rd year	10%–30% of fixed capital		Remaining construction
	+ working capital		
	+ FCOP + 30% VCOP	30% of design basis revenue	Initial production
4th year	FCOP + 50%–90% VCOP	50%–90% of design basis revenue	Shake-down of plant
5th year +	FCOP + VCOP	100% of design basis revenue	Full production at design rates

$$\sum_{n=1}^{n=t} \frac{CF_n}{(1 + i')^n} = 0 \tag{9.21}$$

where: CF_n = cash flow in year n
t = project life in years
i' = the discounted cash flow rate of return (percent /100)

The value of i' is found by trial-and-error calculations or by using the appropriate function (e.g., "goal seek") in a spreadsheet. A more profitable project will be able to pay a higher DCFROR.

DCFROR provides a useful way of comparing the performance of capital for different projects, independent of the amount of capital used, the life of the plant, or the actual interest rates prevailing at any time. DCFROR is a more useful method than NPV when comparing projects of very different sizes. The NPV of large projects is usually greater than that of small projects, but then the investment is also much greater. DCFROR is independent of project size, and the project with the highest DCFROR always provides the best "bang for the buck." When DCFROR is used as an investment criterion, companies usually expect projects to have a DCFROR greater than the cost of capital.

DCFROR can also be compared directly with interest rates. Because of this, it is sometimes known as the *interest rate of return* or *internal rate of return* (IRR).

Example 9.4

Estimate the NPV at a 12% interest rate and the DCFROR for the project described in Example 9.1, using the MACRS depreciation method.

Solution

Calculating the present values of the cash flows from the previous example requires adding two columns to the spreadsheet. We first calculate the discount factor $(1 + i)^{-n}$ and then multiply this by the cash flow in year n to give the present value of the cash flow. The present values can then be summed to give the NPV:

Year	Gross profit (MM$)	Depreciation charge (MM$)	Taxable income (MM$)	Taxes paid (MM$)	Cash Flow (MM$)	Discount factor	Present value of CF (MM$)
0	0	0	0	0	−100	1	−100
1	50	20	30	0	50	0.893	44.64
2	50	32	18	6.30	43.70	0.797	34.84
3	50	19.2	30.8	3.78	46.22	0.712	32.90
4	50	11.52	38.48	6.47	43.53	0.636	27.67
5	50	11.52	38.48	8.08	41.92	0.567	23.79
6	50	5.76	44.24	8.08	41.92	0.507	21.24
7	50	0	50	9.29	40.71	0.452	18.41
8	50	0	50	10.50	39.50	0.404	15.95
9	50	0	50	10.50	39.50	0.361	14.24
10	50	0	50	10.50	39.50	0.322	12.72
				Interest rate		12.00%	
				Total = Net present value =			146.40

Note that we could also have calculated NPV directly using the NPV function. In Microsoft Excel, the NPV function starts at the end of year 1, so any cash flows in year 0 should be added to or subtracted from the result returned by the function and should not be included in the function range.

The DCFROR can then be found by adjusting the interest rate until the NPV is equal to zero. This is easily accomplished in the spreadsheet using the "Goal Seek" tool, giving DCFROR = 44.35%.

Example 9.5

The adipic acid plant from Examples 7.8 and 8.2 is to be built in 2020 with 30% of the fixed investment in year 1 and 70% in year 2, and the plant will operate at 50% of capacity in year 3 before reaching full capacity in year 4. The plant can be depreciated by the straight-line method over 10 years, and profits can be assumed to be taxed at 21% per year, payable the next year. Assume that losses cannot be offset against revenues from other operations for tax purposes (i.e., no tax credits in years when the plant makes a loss). Estimate the following:

1. The cash flow in each year of the project.
2. The simple pay-back period.
3. The NPV with a 15% cost of capital after 10 years of production and after 15 years of production at full capacity.
4. The DCFROR for 15 years of production at full capacity.

Is this an attractive investment?

Solution

The solution requires calculating the cash flows in each year of the project. This is easily coded into a spreadsheet, as illustrated in Fig. 9.2. A blank template of this spreadsheet is given in Appendix G and is available in Microsoft Excel format in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

Company Name
Address

ECONOMIC ANALYSIS
Adipic Acid from Phenol

Form:XXXXX/YY-ZZ

Project Name: Adipic acid from phenol
Project Number
Sheet: 1

REV	DATE	BY	APVD	REV	DATE	BY	APVD
1	1.1.07	GPT					
2	5.6.20	GPT					

Owner's Name
Plant Location: Northeast Asia
Case Description

Capital Cost Basis Year: 2020
Units: Metric
On Stream: 8,000 hr/yr; 333.33 day/yr

REVENUES AND PRODUCTION COSTS

	$MM/yr
Main product revenue	560.0
Byproduct revenue	4.4
Raw materials cost	410.8
Utilities cost	47.3
Consumables cost	13.1
VCOP	466.8
Salary and overheads	16.6
Maintenance	13.0
Interest	3.7
Royalties	3.0
FCOP	36.5

CAPITAL COSTS

	$MM
ISBL Capital Cost	247.9
OSBL Capital Cost	99.2
Engineering Costs	34.7
Contingency	52.1
Total Fixed Capital Cost	433.9
Working Capital	60.9

CONSTRUCTION SCHEDULE

Year	% FC	% WC	% FCOP	% VCOP
1	30%	0%	0%	0%
2	70%	0%	0%	0%
3	0%	100%	100%	50%
4	0%	0%	100%	100%
5	0%	0%	100%	100%
6	0%	0%	100%	100%
7+	0%	0%	100%	100%

ECONOMIC ASSUMPTIONS

Cost of equity	25%	Debt ratio	0.5	Tax rate	21%
Cost of debt	5%			Depreciation method	Straight-line
Cost of capital	15%			Depreciation period	10 years

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project year	Cap Ex	Revenue	COOP	Gr. Profit	Deprcn	Taxbl Inc	Tax Paid	Cash Flow	PV of CF	NPV
1	130.2	0.0	0.0	0.0	0.0	0.0	0.0	-130.2	-113.2	-113.2
2	303.7	0.0	0.0	0.0	0.0	0.0	0.0	-303.7	-229.7	-342.9
3	60.9	280.0	268.9	11.1	43.4	-32.3	0.0	-49.9	-32.8	-375.6
4	0.0	560.0	502.3	57.7	43.4	14.3	0.0	57.7	33.0	-342.7
5	0.0	560.0	502.3	57.7	43.4	14.3	3.0	54.7	27.2	-315.5
6	0.0	560.0	502.3	57.7	43.4	14.3	3.0	54.7	23.6	-291.8
7	0.0	560.0	502.3	57.7	43.4	14.3	3.0	54.7	20.6	-271.3
8	0.0	560.0	502.3	57.7	43.4	14.3	3.0	54.7	17.9	-253.4
9	0.0	560.0	502.3	57.7	43.4	14.3	3.0	54.7	15.5	-237.9
10	0.0	560.0	502.3	57.7	43.4	14.3	3.0	54.7	13.5	-224.3
11	0.0	560.0	502.3	57.7	43.4	14.3	3.0	54.7	11.8	-212.6
12	0.0	560.0	502.3	57.7	43.4	14.3	3.0	54.7	10.2	-202.4
13	0.0	560.0	502.3	57.7	0.0	57.7	3.0	54.7	8.9	-193.5
14	0.0	560.0	502.3	57.7	0.0	57.7	12.1	45.6	6.4	-187.0
15	0.0	560.0	502.3	57.7	0.0	57.7	12.1	45.6	5.6	-181.4
16	0.0	560.0	502.3	57.7	0.0	57.7	12.1	45.6	4.9	-176.6
17	0.0	560.0	502.3	57.7	0.0	57.7	12.1	45.6	4.2	-172.3
18	0.0	560.0	502.3	57.7	0.0	57.7	12.1	45.6	3.7	-168.7
19	0.0	560.0	502.3	57.7	0.0	57.7	12.1	45.6	3.2	-165.5
20	-60.9	560.0	502.3	57.7	0.0	57.7	12.1	106.5	6.5	-159.0

ECONOMIC ANALYSIS

Average cash flow	48.9 $MM/yr	NPV	10 years	-224.3 $MM	IRR	10 years	-1.8%
Simple pay-back period	10.1 yrs		15 years	-181.4 $MM		15 years	5.0%
Return on investment (10 yrs)	1.37%		20 years	-159.0 $MM		20 years	7.2%
Return on investment (15 yrs)	3.63%	NPV to yr	19	-165.5 $MM			

FIG. 9.2 Economic analysis worksheet for Example 9.5.

Cash flow table

In years 1 and 2 of the project there are capital expenses but no revenues or operating costs. The capital expenses are not operating losses and so they have no effect on taxes or depreciation. They are negative cash flows.

In year 3 the plant operates at 50% capacity and generates 50% of the design basis revenue. All of the working capital must be invested. The plant incurs 100% of the fixed cost of production but only 50% of the variable cost. Because the plant makes a profit, depreciation can be charged. Using the straight-line method of depreciation with a 10-year recovery period, the annual depreciation charge is one-tenth of the total fixed capital investment = 433.9/10 = $43.4 MM. Because the gross profit in year 3 is only $11.1 MM, the effect of charging depreciation is that the taxable income is negative and so no taxes are owed in year 4 (taxes are paid based on the previous year's income).

In year 4 the plant operates at full capacity and generates 100% of the design basis revenues with 100% of the VCOP. From here onwards the plant makes a gross profit of $57.7 MM each year.

Depreciation is charged for 10 years (i.e., until year 12). The taxable income therefore increases in year 13 and the taxes paid increase in year 14, giving a reduction in cash flow from $54.7 MM to $45.6 MM.

In the final year of the project, the working capital is released and should be taken as a positive increment to the cash flow. This is shown as occurring in year 20 in Fig. 9.2, but should be adjusted when the length of the project is varied, as described next.

The present value of the cash flow in year n can be found by multiplying by $(1+i)^{-n}$, as stated in Equation 9.19. The NPV up to year n is the cumulative sum of all the present values of cash flow up to that year.

Simple pay-back period

The simple pay-back is calculated from the fixed investment and the average annual cash flow (Equation 9.15). The average annual cash flow should be based only on the years in which the plant generates revenue (i.e., years 3 to 20) and is found to be \$48.9 MM/y. Note that it does not matter if this range includes the year in which working capital is invested, as long as it also includes the year in which working capital is recovered. The working capital thereby cancels out and is not included in the average cash flow.

The simple pay-back period is then found from:

$$\text{simple pay}-\text{back time} = \frac{\text{total investment}}{\text{average annual cash flow}} = \frac{433.9+60.9}{48.9} = \underline{\underline{10.1 \text{ years}}} \tag{9.15}$$

Net present value

The NPV with a 15% cost of capital after 10 years of production is the NPV at the end of year 13. This can be looked up in the cash flow table and is \$−193.5 MM. If the plant is closed after 10 years of production and the working capital is released, there would be an additional cash flow of \$60.9 MM in year 13, increasing the NPV to \$−132.6 MM.

The NPV after 15 years of production is the NPV at the end of year 18, which can also be found from the cash flow table, and is \$−168.7 MM. If the plant is closed after 15 years of production and the working capital is released, there would be an additional cash flow of \$60.9 MM in year 18, increasing the NPV to \$−107.7 MM.

In all cases the NPV for this project is negative, so it is not an attractive investment with a 15% cost of capital. We already knew this would be the case based on the cost of production analysis in Example 8.2, which had shown that the total cost of production (TCOP) with capital recovered at a 15% interest rate was greater than the expected revenue.

Internal rate of return (DCFROR)

The DCFROR (IRR) of the project after 15 years of production at full capacity can be found by either adjusting the interest rate (manually or using the goal seek function) until the NPV at the end of year 18 is equal to zero, or by using the IRR function in the spreadsheet over the range year 1 to year 18. The working capital should be included as a recovered cost in year 18.

The answer obtained in either case is *DCFROR* = 8.03%. This is the maximum interest rate at which this project can be financed to break even in 15 years of production. Note that this is not the same as the IRR at the end of year 15 calculated in Fig. 9.2.

Summary

None of the economic measures indicates that this is an attractive project with the projected costs, revenues, and capital expenses. It should perhaps be noted, though, that this analysis was based on a class 5 estimate of the capital cost (±50%). If we had any technical improvement in mind that could reduce either the capital investment or the cost of production, we might want to develop the design further to assess if the economic analysis was sufficiently improved.

9.7 Annualized cost methods

9.7.1 Amortization charges

An alternative method of comparing the magnitude of a capital investment in current dollars with a revenue stream in the future is to convert the capital cost into a future annual capital charge. A capital cost can be annualized (amortized) by determining the annual payment that is needed to repay the initial investment, together with the expected return on capital in the form of compound interest.

If an amount P is invested at an interest rate i, then after n years of compound interest, it matures to the sum $P\ (1 + i)^n$.

If, instead, an amount A is invested each year, also at interest rate i, then it matures to a sum, S, where:

$$S = A + A(1+i) + A(1+i)^2 + \ldots + A(1+i)^{n-1} \tag{9.22}$$

so:

$$S(1+i) = A(1+i) + A(1+i)^2 + \ldots + A(1+i)^n \tag{9.23}$$

Hence, subtracting Equation 9.22 from Equation 9.23:

$$S\,i = A[(1+i)^n - 1] \tag{9.24}$$

If the annual payments A have matured to give the same final sum as would have been obtained by investing the principal P at the same interest rate, then:

$$S = P(1+i)^n = [(1+i)^n - 1]$$

Hence:

$$A = P\ \frac{[i\ (1\ +\ i)^n]}{[(1\ +\ i)^n\ -\ 1]} \tag{9.25}$$

A is then the regular annual payment that must be made to generate the same amount of money over n years as would be earned by investing P at interest rate i for n years. A is also the annual payment that would have to be paid to pay off (amortize) the principal and interest on a loan of amount P, borrowed at interest rate i, over a term of n years.

We can define an annual capital charge ratio, $ACCR$, as:

$$ACCR = \frac{A}{P} = \frac{[i\ (1\ +\ i)^n]}{[(1\ +\ i)^n\ -\ 1]} \tag{9.26}$$

The ACCR is the fraction of the principal that must be paid out each year to fully repay the principal and all accumulated interest over the life of the investment. This is the same formula used for calculating fixed annual payments on home mortgages and other loans where the principal is amortized over the loan period.

TABLE 9.3 Values of annual capital charge ratio (ACCR) for different interest rates

Interest rate, i	*ACCR:* 10-year life	*ACCR:* 20-year life
0.1	0.163	0.117
0.12	0.177	0.134
0.15	0.199	0.16
0.2	0.239	0.205
0.25	0.280	0.253
0.3	0.323	0.302

9.7.2 Annualized capital cost and total annualized cost

If the cost of capital is used as the interest rate (see Section 9.3.4), then the ACCR can be used to convert the initial capital expense into an annual capital charge, or annualized capital cost:

$$\text{Annual capital charge (ACC)} = ACCR \times \text{total fixed capital cost} \tag{9.27}$$

The annual capital charge can be added to the operating costs to give a total annualized cost of production (TAC):

$$\text{TAC} = \text{operating costs} + ACCR \times \text{total fixed capital cost} \tag{9.28}$$

The TAC can be compared with forecasted future revenues. The TAC is also sometimes referred to as TCOP.

Table 9.3 shows values of *ACCR* for different values of *i* and *n*. For a typical cost of capital of about 15% and a plant life of 10 years, the value of *ACCR* is 0.199, or about one-fifth of the capital investment.

A few important things should be noted when using the annualized cost method:

1. The method assumes investment and cash flows begin immediately, and so it does not capture information on the timing of early expenditures and revenues. In this respect it is inferior to NPV and DCFROR.
2. The method does not take into account taxes or depreciation and assumes that all of the revenue from the project is available to provide a return on the initial investment. The tax and depreciation schedule is not easily annualized if the MACRS system is used.
3. Working capital is recovered at the end of the project and so strictly only the fixed capital should be annualized. Equations 9.25 and 9.26 can be modified for the case where an additional sum becomes available at the end of the investment term, but this modified version is seldom used in practice, and working capital is often either neglected in the annualized cost method or else (wrongly) thrown in with fixed capital. A simple way around this problem is to assume that the working capital is entirely funded by debt, in which case the cost of carrying the working capital is reduced to an interest payment that appears as part of the fixed costs of production. At the end of the project life the working capital will be released and will be available to repay the principal on the debt.
4. As described in Section 8.5, several of the fixed costs of production are proportional to the fixed capital invested (*FC*). If we assume annual charges of 3% of *FC* for maintenance, 2% of *FC* for property tax, and 65% plant overhead, then the annual capital charge ratio is increased by $0.02 + (1.65 \times 0.03) = 0.07$.
5. If we also assume engineering costs are 10% of (ISBL + OSBL) capital investment and add 15% of (ISBL + OSBL) capital as contingency, then with a 10-year plant life and a 15% interest rate, the annual capital charge ratio is:

$$\begin{aligned} ACCR &= [0.199 \times (1.0 + 0.1 + 0.15) + 0.07] \times [\text{Installed ISBL} + \text{OSBL capital cost}] \\ &= 0.32 \times [\text{Installed ISBL} + \text{OSBL capital cost}] \end{aligned} \tag{9.29}$$

Equation 9.29 is the basis for the widely used rule of thumb of annualizing capital cost by dividing by 3. When using this rule of thumb, it is important to remember that some, but not all, of the fixed costs have been counted in the annual capital charge.

The annualized cost method involves more assumptions than calculating NPV or DCFROR, but it is widely used as a quick way of comparing investments with the resulting benefits. Annualized cost is also useful as a method for analyzing small projects and modifications that lead to reduced operating costs (for example, heat recovery projects), because the annualized capital outlay can be directly traded off against the expected annual savings, and there is usually no change in working capital, operating labor, or other fixed costs of production. Small projects usually can be executed quickly, so the error introduced by neglecting the timing of investments and revenues is less important than it is when designing a new plant or a major investment project.

The annualized cost method is also used when comparing the costs of equipment with different expected operating lives. Annualization of the costs allows equipment with different service life to be compared on the same annual basis. This is illustrated in the example that follows.

Example 9.6

A carbon steel heat exchanger that costs $140,000 is expected to have a service life of 5 years before it requires replacement. If type 304 stainless steel is used, then the service life will be increased to 10 years. Which exchanger is the most economical if the cost of capital is 12%?

Solution

With a 12% interest rate and 5-year life, the annual capital charge ratio is

$$ACCR = \frac{[i\ (1\ +\ i)^n]}{[(1\ +\ i)^n\ -\ 1]} = \frac{\left[0.12\ (1.12)^5\right]}{\left[(1.12)^5\ -\ 1\right]} = 0.277 \tag{9.26}$$

The annualized capital cost of the carbon steel exchanger is then $= \$140{,}000 \times 0.277 = \underline{\underline{\$38{,}780/\text{y}.}}$

From Table 7.6, we can estimate the cost of the type 304 stainless steel exchanger to be \$140,000 × 1.3 = \$182,000. From Table 9.3 (or Equation 9.26), with a 10-year life and 12% interest rate, the annual capital charge ratio is 0.177, so the annualized cost of the stainless steel exchanger is:

$$= \$182{,}000 \times 0.177 = \underline{\underline{\$32{,}210/\text{y}}}$$

In this case, it would be more economical to buy the stainless steel heat exchanger.

9.8 Sensitivity analysis

9.8.1 Simple sensitivity analysis

The economic analysis of a project can only be based on the best estimates that can be made of the investment required and the cash flows. The actual cash flows achieved in any year will be affected by changes in raw materials costs and other operating costs and will be highly dependent on the sales volume and price. A sensitivity analysis is a way of examining the effects of uncertainties in the forecasts on the viability of a project. To carry out the analysis, the investment and cash flows are first calculated using what are considered the most probable values for the various factors; this establishes the base case for analysis. Various parameters in the cost model are then adjusted, assuming a range of error for each factor in turn. This will show how sensitive the cash flows and economic criteria are to errors in the forecast figures. A sensitivity analysis gives some idea of the degree of risk involved in making judgments on the forecast performance of the project.

The results of a sensitivity analysis are usually presented as plots of an economic criterion such as NPV or DCFROR vs. the parameter studied. Several plots are sometimes shown on the same graph using a scale from 0.5 × base value to 2 × base value as the abscissa, as illustrated in Example 9.7.

9.8.2 Parameters to study

The purpose of sensitivity analysis is to identify those parameters that have a significant impact on project viability over the expected range of variation of the parameter. Typical parameters investigated and the range of variation that is usually assumed are given in Table 9.4.

Varying the production rate (while keeping investment and fixed costs constant) investigates the effects of unexpectedly high downtime due to maintenance or operations problems, as well as unexpected difficulties in selling the full volume of product that could be produced. An increase in production rate beyond the design capacity might also be possible if the plant design margins allow some extra capacity or if the yields can be improved by use of a better catalyst, etc.

TABLE 9.4 Sensitivity analysis parameters

Parameter	Range of variation
Sales price	±20% of base (larger for cyclic commodities)
Production rate	±20% of base
Feed cost	−10% to +30% of base
Fuel cost	−50% to +100% of base
Fixed costs	−20% to +100% of base
ISBL capital investment	−20% to +50% of base
OSBL capital investment	−20% to +50% of base
Construction time	−6 months to +2 years
Interest rate	base to base +2 percentage points

The choice of which feed and product prices to use in the sensitivity analysis depends strongly on the method of price forecasting that has been used. Typically, total raw material cost is studied rather than treating each feed separately, but if raw material costs are found to be the dominant factor, they may be broken out into the costs of individual raw materials.

9.8.3 Statistical methods for risk analysis

In a simple sensitivity analysis, each parameter is varied individually and the output is a qualitative understanding of which parameters have the most impact on project viability. In a more formal risk analysis, statistical methods are used to examine the effect of variation in all of the parameters simultaneously and hence quantitatively determine the range of variability in the economic criteria. This allows the design engineer to estimate the degree of confidence with which the chosen economic criterion can be said to exceed a given threshold.

A simple method of statistical analysis was proposed by Piekarski (1984) and is described in Humphreys (2005). Each item in the estimate is expressed as a most likely value, *ML*; an upper value, *H*; and a lower value, *L*. The upper and lower values can be estimated using the ranges of variation given in Table 9.4. The mean and standard deviation are then estimated as:

$$\text{mean value, } \overline{x} = \frac{(H + 2ML + L)}{4} \tag{9.30}$$

$$\text{standard deviation, } S_x = \frac{(H - L)}{2.65} \tag{9.31}$$

Note that the mean is not necessarily equal to the most likely value if the distribution is skewed. This is often the case for cost estimates, where the likelihood of costs being underestimated is much greater than the likelihood of them being overestimated.

The mean and standard deviation of other parameters can then be estimated by combination of the individual means and standard deviations using the mathematics of statistics given in Table 9.5.

This allows relatively easy estimation of the overall error in a completed cost estimate, and with a little more difficulty can be extended to economic criteria such as NPV, TAC, or ROI.

Rather than build the simple method noted earlier into a spreadsheet, a more sophisticated approach is to take the economic model and subject it to analysis using Monte Carlo simulation. In Monte Carlo simulation, random numbers are generated and used to establish the value of each parameter within its allowed range. For example, each parameter could be set equal to $L + (R \times (H - L)/10)$, where R is a random number between 1 and 10. The overall probability distribution in the calculated parameter (economic criterion) can be estimated by performing a large number of such simulations. Several commercial programs for Monte Carlo simulation are available, for example REP/PC (Decision Sciences Corp.), @RISK (Palisade Corp.), and CRYSTAL BALL (Decisioneering Corp.).

TABLE 9.5 Mathematics of statistics

If: $y = f(\overline{x}, \overline{z})$, then the standard deviation of y, S_y, is given as a function of S_x and S_z.	
Function y of $\overline{x}$, $\overline{z}$	**Standard deviation S_y**
$y = a\overline{x} + b\overline{z}$	$S_y = \sqrt{a^2 S_x^2 + b^2 S_z^2}$
$y = \overline{x}\,\overline{z}$	$S_y = \overline{x}\,\overline{z}\sqrt{\frac{S_x^2}{\overline{x}^2} + \frac{S_z^2}{\overline{z}^2}}$
$y = \frac{\overline{x}}{\overline{z}}$	$S_y = \frac{\overline{x}}{\overline{z}}\sqrt{\frac{S_x^2}{\overline{x}^2} + \frac{S_z^2}{\overline{z}^2}}$

Notes:

1. *These formulae are strictly true only when the covariance of x and z is zero, that is, there is no statistical interrelation between x and z and x* and *z have been estimated from a small set of data points.*
2. *For a more general description of the formulae, see Ku (1966).*

Care must be taken in formulating Monte Carlo simulation problems. The Monte Carlo method implicitly assumes that all parameters vary randomly and independently. If two parameters are correlated (for example, feedstock and product prices or feedstock and energy prices), they should not be varied independently. The correct approach is to vary one of the parameters and then predict the other by correlation, imposing a smaller random error on the predicted parameter to reflect the accuracy of the correlation.

The cost estimating literature contains a lot of information on risk analysis. Good introductions to the use of statistics in risk analysis are given by Humphreys (2005) and Sweeting (1997). Anderson (2010) gives an overview of the subject and suggests several approaches to presenting the data and results.

9.8.4 Contingency costs

The concept of a contingency charge to allow for variation in the capital cost estimate was introduced in Section 7.2.1, where it was suggested that a minimum contingency charge of 10% of ISBL plus OSBL fixed capital should be used.

If the confidence interval of the estimate is known, the contingency charges can also be estimated based on the desired level of certainty that the project will not overrun the projected cost. For example, if the cost estimate is normally distributed, then the estimator has the following confidence levels:

- 90% confidence that the cost is less than $\overline{x} + 1.3\ S_x$
- 95% confidence that the cost is less than $\overline{x} + 1.65\ S_x$
- 98% confidence that the cost is less than $\overline{x} + 2.05\ S_x$
- 99% confidence that the cost is less than $\overline{x} + 2.33\ S_x$

Although many of the components of a cost estimate are skewed distributions, when these are combined, the resulting distribution is often approximately normal. These guidelines can thus be used to determine the amount of contingency charge needed for a given level of confidence.

Note also that a 10% contingency charge gives 98% confidence of the cost coming in under estimate if the estimate has accuracy ±6.5% (using the approximate method of calculating S_x given in Equation 9.31). This illustrates that a 10% contingency charge should really be viewed as a minimum level and is only appropriate for detailed estimates (Class 1 and Class 2) when the technology is well understood.

Additional guidance on improving estimates of contingency costs is given by Hollmann (2014).

Example 9.7

Carry out a sensitivity analysis on the adipic acid project described in Example 9.5. Investigate the sensitivity of the NPV after 10 years of production to variation in total fixed capital (−20% to +50%), annual gross profit (−20% to +30%), and project construction schedule (−6 months to +1.5 years).

Solution

Because the economic analysis is entered in a spreadsheet, it is easy to investigate the effect of varying any parameter. The simplest method is to define a ratio parameter in an empty cell and then multiply the cell or cells of interest by this ratio. The ratio can then be varied and the effect on NPV tabulated. For fixed capital, the ratio varies from 0.8 to 1.5, and for annual gross profit, the ratio varies from 0.8 to 1.3.

The effect of variation in the project schedule is a little more difficult. The easiest way to study this is to change the numbers in the construction schedule section of the worksheet. It is usually a good idea to set up the economic analysis with the construction schedule as a defined parameter (as in Fig. 9.2) so that the effect of changes in schedule can be studied. For the purposes of this example it was assumed that a 1-year delay in schedule would mean the project would still incur 100% of fixed costs in year 3, but would achieve 50% of revenues and variable costs in year 4 instead of year 3. A 6-month delay would then give 25% of revenues and variable costs in year 3 and 75% in year 4, etc. A 6-month acceleration in schedule was assumed to bring 25% of revenues and variable costs into year 2, 75% of revenues and variable costs in year 3, and 100% of working capital and 50% of fixed costs into year 2 to allow for hiring staff and beginning production sooner.

The results can be plotted on the same graph for all three variables. For a base case schedule of 3 years, a 6-month reduction is 2.5/3 = 83% of base case. A 1.5-year delay would be 4.5/3 = 150% of base case.

The results are shown in Fig. 9.3. It can be seen that none of the parameters studied can cause the project to have positive NPV over the expected range of variation. The project economics are more sensitive to capital investment (CAPEX) and gross profit than to schedule. Gross profit usually depends on market conditions and cannot be controlled for a commodity such as

adipic acid. The investors in this project should therefore concentrate their efforts on driving down capital cost rather than trying to accelerate the schedule.

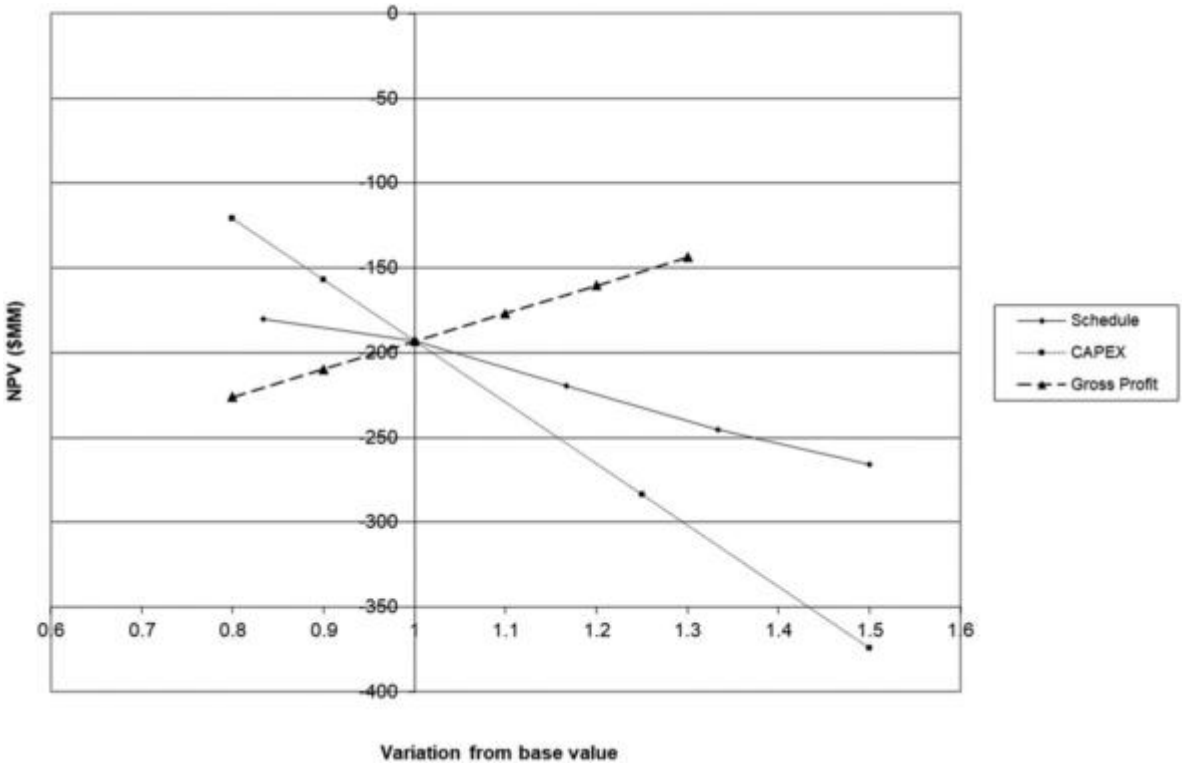


FIG. 9.3 Sensitivity analysis for Example 9.7

Example 9.8

A preliminary (Class 4) estimate of the ISBL capital cost of building a 200,000 ton per year ethanol plant by corn dry milling has been stated as \$130 MM −30% / +50%. The plant is to be built on a greenfield site, and offsite costs are estimated to be between \$40 MM and \$60 MM. Estimate a value for the total project cost that will give 98% confidence that the project can be carried out within the amount estimated.

Solution

For the ISBL cost, $H = \$195$ MM, $L = \$91$ MM, and $ML = \$130$ MM, so:

$$\bar{x}_{ISBL} = \frac{(H + 2ML + L)}{4} = \frac{(195 + 260 + 91)}{4} = \$136.5 \text{ MM} \tag{9.30}$$

$$S_{x,ISBL} = \frac{(H - L)}{2.65} = \frac{195 - 91}{2.65} = \$39.2 \text{ MM} \tag{9.31}$$

Similarly, for the OSBL costs, assuming the most likely value is in the middle of the range given:

$$\bar{x}_{OSBL} = \frac{(H + 2ML + L)}{4} = \frac{(40 + 100 + 60)}{4} = \$50 \text{ MM} \tag{9.30}$$

$$S_{x,OSBL} = \frac{(H - L)}{2.65} = \frac{60 - 40}{2.65} = \$7.55 \text{ MM} \tag{9.31}$$

Both mean values should be increased by 10% to allow for engineering costs, so combining the means gives:

$$\bar{x}_{Total} = 1.1\,\bar{x}_{ISBL} + 1.1\,\bar{x}_{OSBL} = \$205.2 \text{ MM}$$

$$S_{x,Total} = \sqrt{(1.1\,S_{x,ISBL})^2 + (1.1\,S_{x,OSBL})^2} = \$43.9 \text{ MM}$$

We have 98% confidence that the cost is less than $\bar{x} + 2.05\, S_x = 205.2 + (2.05 \times 43.9) = \$295$ MM. If we budget the project for this amount (or tender a contract), then we are accepting a 1 in 50 risk that the project will exceed the given budget. Note that this is substantially larger than the most likely value of $1.1 \times 180 = \$198$ MM, showing the impact of the high error in a Class 4 estimate. The required contingency to give 98% confidence is $295 - 198 = \$97$ MM, or 49% of the most likely estimate.

Example 9.9

If the capital costs in the adipic acid example described in Example 9.5 are known to within −10% to +30% and the cash flow from operations is predicted within ±10%, estimate the mean and standard deviation of the NPV after 10 years of production. Is there a greater than 1% likelihood of the NPV being greater than zero?

Solution

Once again, the spreadsheet is easily extended to calculate the statistical parameters.

In years 1 and 2, the cash flows are only associated with capital expense and are all negative. We can therefore use the present value of cash flow as the most likely value (*ML*) and estimate the lower bound (*L*) as $1.3 \times ML$ (because we know the numbers are negative) and the upper bound (*H*) as $0.9 \times ML$.

In years 4 to 13, the cash flows are only positive and associated with operations. We can use the present value of cash flow as the value of *ML* and then estimate $L = 0.9 \times ML$ and $H = 1.1 \times ML$.

Year 3 is a little more complex, as the cash flow has contributions from both capital outlays and income from operations. The most likely value is still the value previously predicted (−34.0). The low value (*L*) will be the present value of 90% of the gross profit minus 130% of the capital expense:

$$\frac{(0.9 \times 12.8) - (1.3 \times 59.6)}{(1.15)^3} = -43.3$$

Similarly, the high value (*H*) will be the present value of 110% of the gross profit minus 90% of the capital expense.

We can then tabulate the values of *ML*, *H*, and *L* and calculate the mean and standard deviation using Equations 9.30 and 9.31, as in Table 9.6.

TABLE 9.6 Solution to Example 9.9

Year	*ML*	*L*	*H*	*x*	*S*	S^2
1	−113.19	−147.15	−101.87	−118.85	17.09	291.93
2	−229.67	−298.57	−206.70	−241.15	34.67	1201.80
3	−32.59	−45.29	−27.86	−34.58	6.58	43.26
4	33.01	29.71	36.31	33.01	2.49	6.21
5	27.21	24.49	29.93	27.21	2.05	4.22
6	23.66	21.29	26.03	23.66	1.79	3.19
7	20.57	18.52	22.63	20.57	1.55	2.41
8	17.89	16.10	19.68	17.89	1.35	1.82
9	15.56	14.00	17.11	15.56	1.17	1.38
10	13.53	12.17	14.88	13.53	1.02	1.04
11	11.76	10.59	12.94	11.76	0.89	0.79
12	10.23	9.21	11.25	10.23	0.77	0.60
13	8.89	8.01	9.78	8.89	0.67	0.45
			Sum	−212.27		1559.09
			S		39.5	

The overall mean NPV is the sum of the mean values = $−212.3 MM

The standard deviation is the root of the sum of squares of the S_x values (see Table 9.5) = $39.5 MM.

The 99% confidence interval is $\bar{x} + 2.33\ S_x$, so we have 99% confidence that the NPV will be less than $−212.3 + (2.33 \times 39.5) = \$-120.3$ MM. The design team can state that there is less than 1% probability of this project delivering an NPV greater than $−120 million at 15% cost of capital after 10 years of production.

9.9 Project portfolio selection

A typical company involved in the chemical, pharmaceutical, or fuels industries will evaluate many projects each year. Only a few of these projects are selected for implementation. This section discusses some of the criteria and methods used in making that selection.

9.9.1 Types of projects

Investment projects are carried out for a variety of reasons.

Regulatory compliance projects are often required as a result of changes in environmental or other legislation. If the government changes the rules on plant safety, emissions, or product specifications, then unless an exemption can be obtained, the plant must be modified or closed down. Regulatory compliance projects often have poor financial performance unless the costs of going out of business are considered.

Cost reduction projects are aimed at reducing the cost of production of an existing plant. The most common cost reduction investments are for *preventive maintenance*, in which equipment is replaced, repaired, or cleaned after a planned interval and before the equipment deteriorates to the point where it could affect process performance or safety. Most preventive maintenance projects are small and are handled through the plant maintenance budget, but some can be very large, expensive projects requiring a major plant shutdown, for example, replacing the fired tubes in a main plant furnace. Another common type of cost reduction project is *heat recovery* or *heat integration projects*, in which the plant heat exchange network or utility system is upgraded to reduce energy costs.

Whenever possible, companies also seek to fund *growth projects* that can be expected to give high returns on the capital invested. Growth projects include expansions of existing units, often referred to as *debottlenecking* or *revamp projects*, as well as construction of entirely new plants in *grassroots projects*.

In all cases except grassroots projects, a large amount of information about the existing plant, site, and products is usually needed before the project can be designed. Much effort is typically spent on reconciling simulation or other models to the plant performance so as to make the models useful for designing the plant modifications.

Grassroots projects are typically used as undergraduate design projects because they are self-contained and do not require model reconciliation; however, in industrial practice, they make up less than 10% of all projects.

9.9.2 Limits on the project portfolio

The most obvious limit on the portfolio of projects that can be funded is the availability of capital, which is in turn limited by the financing arrangements of the company (see Section 9.3).

Capital spending is often set in proportion to sales, operating profit, or total assets. Table 9.7 shows recent information on capital spending for some of the largest chemical companies in the world. These capital expenditures are plotted against revenues in Fig. 9.4 and against total assets in Fig. 9.5. Although the figures show that the correlation is not particularly strong, it can be seen from Table 9.7 that most of the companies' capital spending was between 5% and 10% of sales (mean 7.7%) and also between 4% and 8% of assets (mean 6.2%).

A second important constraint on the number of projects that can be carried out is the availability of critical resources. A company with a small engineering staff will only be able to carry out a few projects at one time. Even if extensive use is made of EPC contractors, the owners will still need to provide some engineering support to each project. The availability of EPC contractors can also be an issue during times of peak industry construction. Projects that require extensive research and development work may be delayed because of constraints on the availability of researchers and pilot plant facilities.

Often the most important constraint is set by regulatory timelines. Regulatory compliance projects must be completed in time for the plant or product to comply with the new law. This may dictate a narrow window of typically less than 5 years in which the project must be planned, designed, and constructed, giving the company little choice on when the project must be begun.

Regulatory timelines are extremely important for pharmaceutical products. A new drug is protected by patent for 20 years from the date the patent is filed. Beyond that time, competitors are able to sell generic versions of the drug, and the price usually falls significantly. Before a new drug can be marketed, both the product and the manufacturing process must be approved by the FDA. Pharmaceutical manufacturers thus seek to maximize the revenue that they can obtain from a drug between FDA approval and patent expiration. This requires making advance preparations during the approvals process so that the rate of production can be ramped up quickly when final approval is obtained. The portfolio of investment projects for a pharmaceutical company will be strongly influenced by the expected outcomes of the regulatory approval process for new products.

9.9.3 Decision criteria

There is no single best criterion for economic evaluation of projects. Each company uses its own preferred methods and sets criteria for the minimum performance that will allow a project to be funded. The design engineer must be careful to ensure that the method and assumptions used are in accordance with company policy and that projects are compared on a fair basis. Projects should always be compared using the same economic criterion, but do not have to be compared on *the exact same* basis, because in a global economy there may be significant regional advantages in feed and product pricing, capital costs, labor costs, financing, or investment incentives. Different economic criteria may be used depending on the type of project, although the same criterion must always be used when comparing alternative projects of the same type.

As well as economic performance, many other factors have to be considered when evaluating projects, such as:

1. Safety
2. Environmental problems (waste disposal)
3. Political considerations (government policies and incentives)
4. Location of customers and suppliers (supply chain)
5. Availability of appropriately trained and skilled labor and supporting services
6. Corporate growth strategies
7. Company experience in the particular technology

Some of these factors are discussed in more detail in the discussion of site selection and design in Chapter 11.

Different projects will have different levels of risk, and management must decide whether the potential financial reward is sufficient to justify taking on the associated risks. For example, projects that use new technology or projects located in countries that may be politically unstable have higher risk and would normally require a higher economic impact than less risky investments.

At the plant or site scale, management may have been given a small discretionary capital budget that can be used for preventive maintenance and cost reduction projects (if it is not swallowed up by regulatory compliance projects). These projects are often ranked using simple measures such as pay-back, ROI, or TAC. For a project to be considered for funding, it must meet a minimum (or maximum) criterion, known as a *hurdle rate.* For example, a company may dictate that projects should not be funded unless the pay-back period is less than 2 years. Regulatory compliance projects are often evaluated based on minimum incremental TAC, because it is implicitly assumed that there will be no additional revenue. If there is additional revenue, for example, from sale of a by-product, then this can be offset against the costs. If the cost of compliance is excessive, the alternative costs of closing down or selling the site will also be evaluated.

Small projects or modifications to ongoing projects are often evaluated based on an "incremental ROI" defined as:

$$\text{Incremental ROI} = \frac{\text{incremental profit}}{\text{incremental investment}} \times 100\% \tag{9.32}$$

A separate hurdle rate is set for incremental ROI to ensure that modifications to a large project pay out in their own right and do not get funded just because of the attractiveness (or size) of the base project. This helps prevent creep of project expenses.

Major growth and expansion projects that require significant investment are usually evaluated at the corporate level. Most companies look at the IRR or DCFROR, the fixed and working capital, and the NPV with the interest

TABLE 9.7 Capital spending of large chemical companies

Company	Sales (MM$)	Net profit (MM$)	Total assets (MM$)	Capital spending (MM$)	Capital/sales	Capital/met profit	Capital/assets
DowDuPont	85,977	8412	188,030	3837	0.045	0.456	0.020
BASF	74,066	7462	102,288	4602	0.062	0.617	0.045
Sinopec	69,210	3929	23,735	2962	0.043	0.754	0.125
Sabic	42,120	9518	79,751	3866	0.092	0.406	0.048
ExxonMobil Chemical	32,443	4162	36,035	1494	0.046	0.359	0.041
LyondellBasell Industries	30,783	,615	12,477	1846	0.060	0.329	0.148
Mitsubishi Chemical	28,747	2382	39,915	1883	0.066	0.791	0.047
LG Chem	25,637	2043	26,330	3838	0.150	1.879	0.146
Air Liquide	24,322	2379	45,312	2605	0.107	1.095	0.057
Evonik Industries	17,755	2078	23,968	1220	0.069	0.587	0.051
Covestro	17,273	2982	13,099	835	0.048	0.280	0.064
Bayer	16,859	3708	90,769	1217	0.072	0.328	0.013
Sumitomo Chemical	16,081	1182	18,576	1171	0.073	0.991	0.063
Braskem	15,885	2250	16,212	741	0.047	0.329	0.046
Lotte Chemical	15,051	1790	18,921	1680	0.112	0.939	0.089
Linde PLC	14,900	2244	93,386	1883	0.126	0.839	0.020
Shin-Etsu Chemical	14,439	3657	27,525	2054	0.142	0.562	0.075
Mitsui Chemicals	13,432	846	13,597	482	0.036	0.570	0.035
Solvay	13,353	1606	25,999	817	0.061	0.509	0.031
Yara	12,928	402	16,656	1336	0.103	3.323	0.080
DSM	10,951	1446	16,120	668	0.061	0.462	0.041
Indorama	10,747	903	11,739	506	0.047	0.560	0.043
Asahi Kasei	10,654	1174	13,517	785	0.074	0.669	0.058
Arkema	10,418	1171	11,949	698	0.067	0.596	0.058

Notes:

1. Source: Tullo (2019).
2. Numbers are based on 2018 financial data.

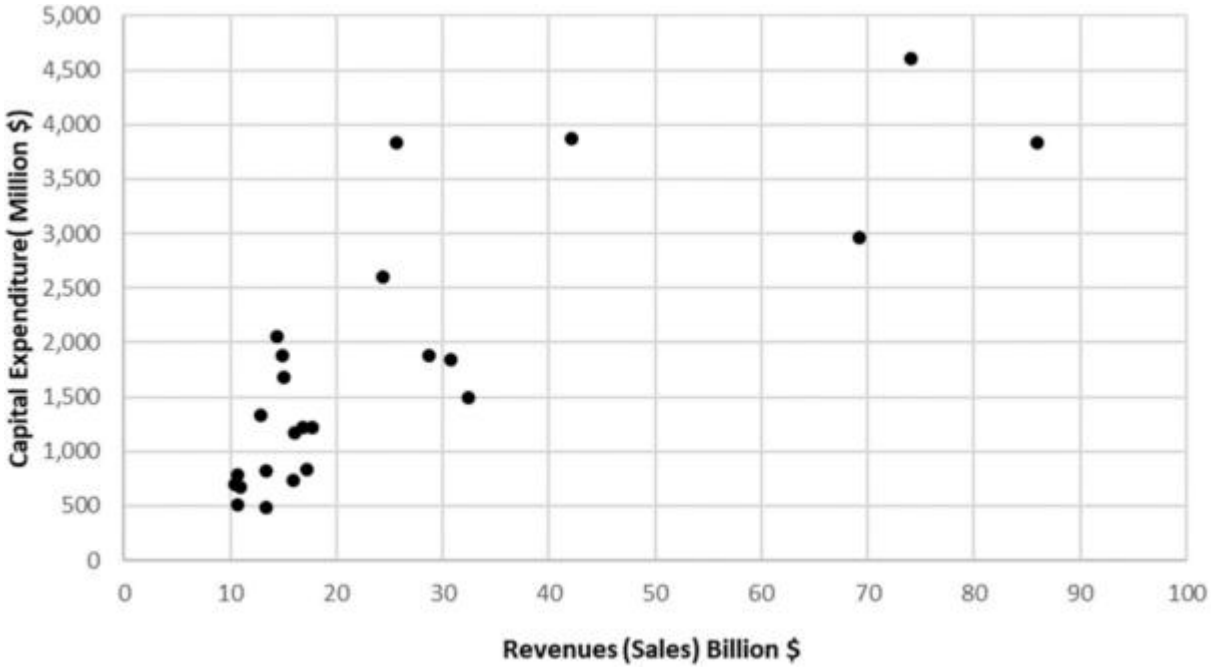


FIG. 9.4 Capital expenditure of major chemical companies versus revenues.

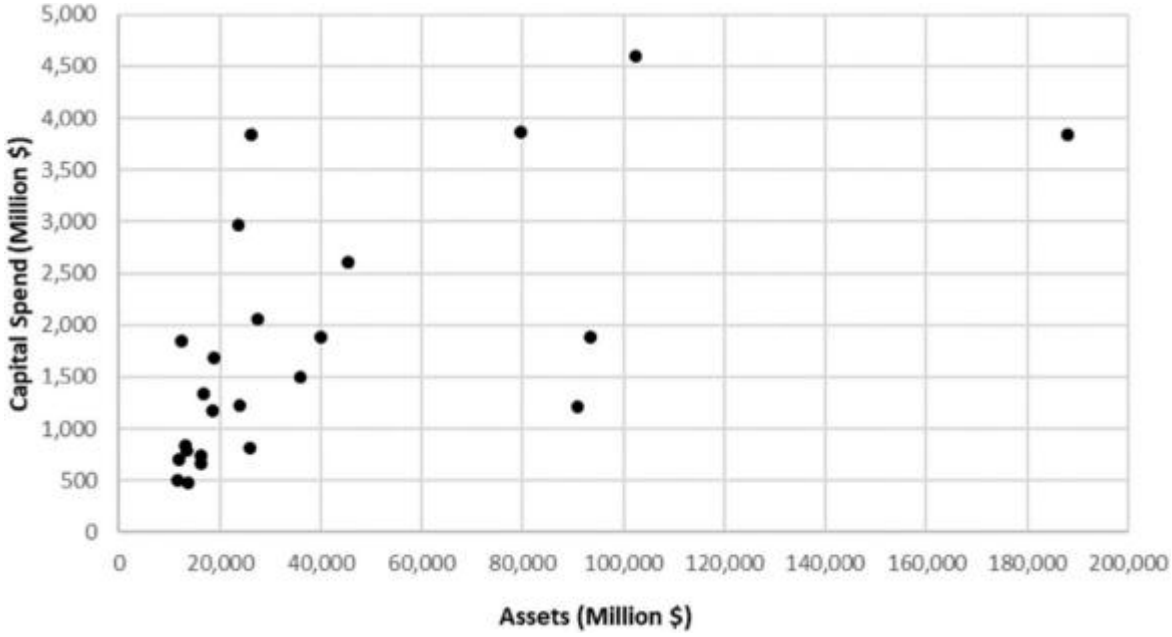


FIG. 9.5 Capital expenditure of major chemical companies versus assets.

rate set equal to the cost of capital. The selection of projects is constrained by the factors described in Section 9.9.2. The set of projects chosen may also be strongly influenced by strategic factors such as the desire to expand a particular business or product line, or a desire to expand the presence of the company in a region that is experiencing rapid economic growth, such as India, China, the Middle East, or Latin America.

Two means of simplifying the selection problem are usually used so that the company's senior management is not faced with a list of thousands of potential projects. The first is to set internal hurdle rates based on simple measures such as IRR or pay-back so that unattractive projects are weeded out at an early stage of the evaluation process. The second method is to divide the available capital budget into categories (sometimes referred to as *buckets*) so as to balance the competing needs of different regions and businesses, growth areas vs. established products, etc. The

various strategic business units or regional subsidiaries (depending on how the company is organized) each submit their proposed capital budgets and a ranked list of projects. Corporate senior management then makes strategic adjustments between the different categories and determines where to draw the line in each list such that the overall portfolio is balanced in accordance with the strategic objectives that they have set for the company. In a large corporation, this process may be repeated at two or more levels of management, with the list of selected projects being passed up to a higher level for further review and approval before the capital is authorized.

The problem of portfolio selection is easily expressed numerically as a constrained optimization: maximize economic criterion subject to constraint on available capital. This is a form of the "knapsack problem," which can be formulated as a mixed-integer linear program (MILP), as long as the project sizes are fixed. (If not, then it becomes a mixed-integer nonlinear program.) In practice, numerical methods are rarely used for portfolio selection, as many of the strategic factors considered are difficult to quantify and relate to the economic objective function.

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9.11 Nomenclature

		Dimensions in $MLT\theta$
A	Annual amount invested	**$**
ACC	Annual capital charge	**$**
ACCR	Annual capital charge ratio	—
B_m	Book value in after m years of depreciation	**$**
C	Capital cost	**$**
C_d	Depreciable value	**$**
CF	Cash flow	**$**
CF_n	Cash flow in year n	**$**
D	Sum of tax allowances, depreciation	**$**

		Dimensions in $MLT0
D_i	Depreciation charge in year i	**$**
DR	Debt ratio (leverage)	—
FC	Fixed capital cost	**$**
F_d	Fraction of book value depreciated each year in declining balance method	—
H	High value of range	**$**
I	Taxable income	**$**
i	Interest rate	—
i'	Discounted cash flow rate of return (internal rate of return)	—
i_c	Cost of capital	—
i_d	Interest rate due on debt	—
i_c	Cost of equity	—
L	Low value of range	**$**
ML	Most likely value of range	**$**
m	Number of years	**T**
NPV	Net present value	**S**
n	Number of years	**T**
P	Gross profit, or principle invested in equations 9.22 to 9.26	**$**
R	Random number between 1 and 10	—
ROA	Return on assets	—
ROE	Return on equity	—
ROI	Return on investment	—
S	Matured sum	**$**
S_x	Standard deviation	**$**
TAC	Total annualized cost	**$**
TCOP	Total cost of production	$\mathbf{\$M^{-1}}$ or $\mathbf{\$T^{-1}}$
t	Time, project life in years	**T**
t_r	Tax rate	—
$\bar{x}$	Mean value	**$**

9.12 Problems

9.1. What annual payment is needed to amortize a loan of $25 million at 7.5% interest over a 20-year period?

9.2. A plant is proposing to install a combined heat and power (CHP) system to supply electrical power and process steam. Power is currently taken from a utility company, and steam is generated using on-site boilers. The capital cost of the CHP plant is estimated to be $23 million. CHP is expected to give net savings of $10 million per year. The plant is expected to operate for 10 years after the completion of construction. Calculate the cumulative net present value of the project at a discount rate of 12% using MACRS depreciation with a 7-year recovery term. Also calculate the discounted cash flow rate of return.

Construction will take 2 years, and the capital will be paid in two equal increments, at the end of the first and second years. The savings (income) can be taken as paid at the end of each year. Production will start on the completion of construction.

9.3. A process heat recovery study identifies five potential modifications, none of which are mutually exclusive, with the costs and energy savings given here.

Project	Capital cost (MM$)	Fuel savings (MMBtu/hr)
A	1.5	15
B	0.6	9
C	1.8	16
D	2.2	17
E	0.3	8

If fuel costs $6/MMBtu and the plant operates for 350 days/year, which projects have a simple pay-back period less than 1 year?

What is the maximum 10-year NPV that can be achieved with a 15% interest rate and a 21% tax rate? Assume all the projects can be built immediately, and use MACRS depreciation with a 5-year recovery term. What combination of projects is selected to meet the maximum NPV?

9.4. An electronics company wants to fit a solvent recovery system on the vent gas from its circuit board manufacturing line. The solvent recovery system consists of a chiller, a knockout drum, and an adsorbent bed. The adsorbent is periodically regenerated by circulating hot air over the bed and to the chiller and knockout. After consultation with equipment vendors, the following purchased prices are estimated for the major plant equipment:

Item	Cost ($)
Chiller	4000
Knockout drum	1000
Packaged refrigeration plant	3000
Adsorbent vessel (×2)	1500 each
Air blower	4000
Air heater	3000

Estimate the ISBL cost of the plant and the total project cost. If the annual operating costs are $38,000 and the annual savings in recovered solvent are $61,500, what is the IRR of this project?

9.5. A shell and tube heat exchanger is to be used in a corrosive service. If carbon steel tubes are used, the cost of the exchanger is estimated to be $160,000, and it is expected that the exchanger will need to be replaced after 2 years. If stainless steel tubes are used, the service life will be increased to 5 years, but the cost increases to $400,000. If the cost of capital is 15%, which option should be selected?

9.6. The adipic acid plant described in Examples 9.5 and 9.9 is to be built in China, with a location factor of 0.85 and a tax rate of 25%. The cost estimate needs to be updated from 2006 to 2022. Up to 45% of the total investment can be secured as a low-cost loan at an interest rate of 1%.

1. What is the cost of capital if the cost of equity is 40%?
2. What is the NPV for 15 years of production?
3. What is the IRR if the debt must be amortized over 15 years as a fixed cost of production?

9.7. A Class 2 estimate of the ISBL capital cost of building a 200,000 MMlb/yr ethylene cracking plant has been stated as $850 MM −5% / +10%. The plant is to be built as an expansion of an existing site, and off-site costs are estimated to be between $170 MM and $250 MM. Estimate a value for the total project cost that will give 98% confidence that the project can be carried out within the amount estimated.

9.8. Find the most recent annual report for a publicly traded company in the process industries. These are readily available online from company websites. Review the balance sheet, income statement, and cash flow statement and answer the following questions:

1. What fraction of assets is in property plant and equipment?
2. What fraction of assets is tied up in working capital (inventories, supplies, and receivables)?
3. What are the relative values of stockholders' equity and the market value (capitalization) of the company? Can you explain the difference?
4. What fraction of revenues is costs of production? What fraction is selling, general, and administrative (SG&A) overhead? What fraction is R&D costs? What is the overall gross margin of the company, and what do these numbers tell you about the company and the segment of industry it serves?
5. How much cash came in from operations? How much was invested in property, plant, and equipment? How much cash was brought in from financing (or how much was spent on acquiring shares, paying debt, paying dividends, etc.)? What do these numbers tell you about the financial priorities of the company?

(Note to instructors: This problem can be set as an individual or group exercise. It can be very educational to assign different companies to different students or groups and have them present the results orally.)

CHAPTER

10

Safety and loss prevention

KEY LEARNING OBJECTIVES

- The importance of safety in the design and operation of chemical plants
- Safety legislation with which companies must comply
- Standards and codes of practice that help ensure safer designs
- Process and materials hazards that must be considered in design
- Methods such as HAZOP, FMEA, and quantitative risk analysis that are used to analyze and quantify process hazards
- How relief valves are designed and used to prevent failure of vessels due to overpressure

10.1 Introduction

The safe design and operation of facilities is of paramount importance to every company that is involved in the manufacture of fuels, chemicals, and pharmaceutical products.

Any organization has a legal and moral obligation to safeguard the health and welfare of its employees and the general public. Safety is also good business; the good management practices needed to ensure safe operation also ensure efficient operation.

The term *loss prevention* is an insurance term, the loss being the financial loss caused by an accident. This loss will not only be the cost of replacing the damaged plant, paying fines, and settling third-party claims but also the loss of earnings from lost production and lost sales opportunity. In the event of a major incident, such costs can be large enough to overwhelm a company.

All manufacturing processes are hazardous to some extent, but in chemical processes there are additional, special, hazards associated with the chemicals used and the process conditions. The designer must be aware of these hazards and ensure, through the application of sound engineering practice, that the risks are reduced to tolerable levels.

In this chapter the discussion of safety in process design will of necessity be limited. A more complete treatment of the subject can be found in the books by Wells (1996) (1997), Mannan (2012), Fawcett and Wood (1982), Green (1982), Crowl and Louvar (2019), Cameron and Raman (2005), and Carson and Mumford (1988, 2002) and in the general literature, particularly the publications by the American Institute of Chemical Engineers and the Institution of Chemical Engineers. The proceedings of the symposia on safety and loss prevention organized by these bodies also contain many articles of interest on general safety philosophy, techniques and organization, and the hazards

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associated with specific processes and equipment. A good general overview of safety issues in process design is given in the AIChE Center for Chemical Process Safety book *Guidelines for Engineering Design for Process Safety* (CCPS, 2012). The Institution of Chemical Engineers has published a book on safety of particular interest to students of chemical engineering: Marshall and Ruhemann (2000).

Although an effort has been made to provide a summary of the major legal requirements and relevant codes and standards, the area of process safety undergoes continuous improvement and many of the standards are rewritten annually, so the information presented here may not be current by the time of publication. Updated information can be obtained from the standards organizations and regulatory agencies. The design engineer should always consult the most recent version of the laws, regulations, or standards and should always make a thorough check to ensure that the design complies with all local regulations and current best practices.

10.1.1 Safety legislation

Because of the particular hazards associated with processing large quantities of chemicals and fuels, most governments have enacted legislation to ensure that the best safety practices are followed. In the United States, the major federal laws relating to chemical plant safety are:

1. The Occupational Safety and Health Act, 29 U.S.C. 651 *et seq.* (1970): Employers must provide a place of employment free from recognized hazards to safety and health, such as exposure to toxic chemicals, excessive noise, mechanical dangers, heat or cold stress, or unsanitary conditions. Employers must provide personal protective equipment and training, including communication of hazards. Facilities must undergo hazard analysis. The Occupational Safety and Health Administration (OSHA) is established to promote best practices, inspect facilities, set standards, and enforce the law.
2. The Toxic Substances Control Act (TSCA), 15 U.S.C. 2601 *et seq.* (1976): The Environmental Protection Agency (EPA) is required to regulate the 75,000 chemical substances used in industry. Extensive review is required before a new chemical can be manufactured, imported, or sold in the United States. The EPA can ban or restrict the import, manufacture, and use of any chemical. Under TSCA, anyone has a right and an obligation to report information about new or alleged health or environmental effects caused by a chemical. Companies must submit a premanufacture notice (PMN) to the EPA 90 days before manufacturing or importing a new chemical. In 2016 TSCA was amended by the Frank R. Lautenberg Chemical Safety for the 21st Century Act, which introduced additional requirements around risk-based chemical assessments, public transparency for chemical information, and enforceable deadlines for the EPA to evaluate the safety of existing chemicals in commerce.
3. The Emergency Planning and Community Right-to-Know Act (EPCRA), 42 U.S.C. 11001 *et seq.* (1986): Facilities must make plans for major incidents. Plans must be made public to the local community.

In addition, releases of material to the environment as a result of loss of containment during an incident are prohibited by various environmental laws. These are discussed in Chapter 11.

Various states, municipalities, and other bodies may also enact legislation that regulates the safe operation of chemical plants (for example, local fire codes). Local regulations may place stricter requirements on the design and operation of facilities but do not absolve the owner or designer from obligations under national or federal laws.

The most recent version of local, national, and federal laws and standards must always be consulted during design. The requirements for legal compliance may change over time due to revisions of legislation, court actions, or executive orders. The design engineer should be aware of the relevant legislation, but is not usually expected to interpret the requirements of the law and will usually rely upon corporate lawyers and professional safety experts to set company policies, codes, and standards that ensure legal compliance. If the design engineer has any concerns that corporate policies are not meeting regulatory requirements, these concerns should immediately be raised with management, and if there is no satisfactory response, with the regulatory agencies.

In Canada, the major safety legislation is:

1. The Canadian Centre for Occupational Health and Safety Act (R.S.C., 1985, c. C-13) (1978): Created the Canadian Centre for Occupational Health and Safety (CCOHS) to promote health and safety in the workplace, establish and maintain safety standards, develop programs to reduce or eliminate occupational hazards, and collect statistics.
2. The Canadian Oil and Gas Operations Act (R.S.C., 1985, c. O-7): The National Energy Board and chief safety officer shall review installations, equipment, operating procedures, and personnel before authorizing any oil or gas production activity.

3. The Hazardous Products Act (R.S., 1985, c. H-3): Prohibits the advertising, sale, and import of hazardous products. Requires Workplace Hazardous Materials Information System (WHMIS) labels and Material Safety Data Sheets (MSDS) for chemicals. Allows inspection of facilities for compliance.
4. The Canadian Environmental Protection Act (S.C. 1999, c.33): Establishes a list of toxic substances (sec. 90). The list is given as Schedule 1 of the act.

In this book, only the particular hazards associated with chemical and allied processes will be considered. The more general hazards present in all manufacturing processes, such as the dangers from rotating machinery, falls, falling objects, use of machine tools, and of electrocution, will not be considered. General industrial safety and hygiene are covered in several books: King and Hirst (1998), Asfahl and Rieske (2018), and Channing (2013).

10.1.2 Layers of plant safety

Safety and loss prevention in process design can be considered under the following broad headings:

1. Identification and assessment of the hazards.
2. Control of the hazards: for example, by containment of flammable and toxic materials.
3. Control of the process: prevention of hazardous deviations in process variables (pressure, temperature, flow) by provision of automatic control systems, interlocks, alarms and trips, together with good operating practices and management.
4. Limitation of the loss, the damage and injury caused if an incident occurs: pressure relief, plant layout, and provision of firefighting equipment.

Another way of expressing this is in terms of layers of plant safety, illustrated in Fig. 10.1. Each of the layers in Fig. 10.1 can be activated if the lower levels have all failed.

The most basic level of plant safety is safe process and equipment design. If the process is inherently safe (see Section 10.1.3) incidents are much less likely to occur. The process equipment is the primary means for containing the chemicals that are being processed, as well as keeping out air, and containing high temperatures and pressures. Vessel design codes and standards incorporate safety margins for equipment to reduce the risk of it failing in operation (see Chapter 14). Most countries require chemical plants to be built and operated in accordance with national or industry standards.

The basic process control system (BPCS) should be designed to maintain the plant under safe conditions of temperature, pressure, flow rates, levels, and compositions. In most continuous plants the process control system will attempt to maintain the process within reasonable bounds of a steady-state condition. In batch or cyclic processes, the variation of process parameters ("ramping") will be controlled to occur at a safe rate to prevent overshooting.

If a process variable falls outside of the safe operating range, this should trigger an automatic alarm in the plant control room. The purpose of the alarm is to warn the process operators of the triggering condition so that the operators can intervene accordingly. Care should be taken when designing the plant control system not to include too many alarms and to clarify the necessary operator responses, because too many alarms can overwhelm the

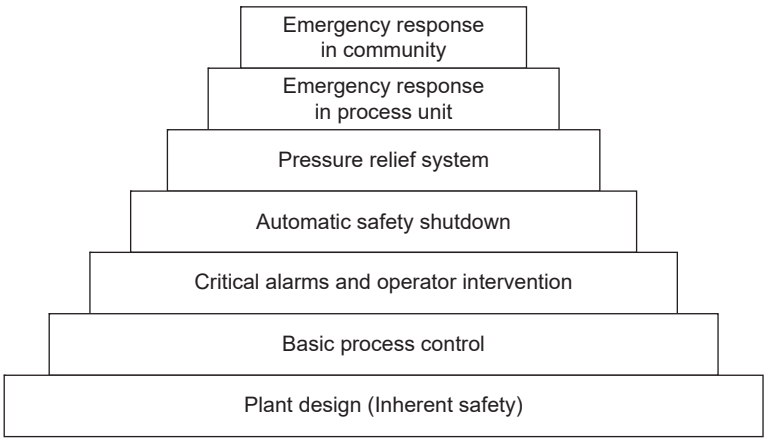


FIG. 10.1 Layers of plant safety.

operators and increase the likelihood of human error (see Section 10.3.7). Alarms should be set so that they are not frequently triggered by normal process variability (in which case they will tend to be ignored) and to allow time for the operator to respond before the next safety layer is activated. See Chapter 5 for more discussion of process control and instrumentation.

In the event that process operators are unable to bring the process back into control when there is a significant deviation of a variable that indicates a hazardous condition, an automatic shut-down of the process (also known as a *trip*) should be activated. Trip systems are sometimes activated by the plant control system and sometimes self-actuated, as described in Chapter 5. Emergency shut-down will usually involve shutting off feeds and sources of heat, depressurizing the process, and purging the plant with inert material. When designing the emergency shut-down procedures and systems, care must be taken to ensure that unsafe conditions are not created or worsened. For example, in some high-temperature or exothermic processes, it may be safer to continue feed of one of the reagents while shutting off the others, so as to remove heat from the reactor. Closing all the valves in a plant is almost never the safest means of shutting it down. A good guide to the design of control, alarm, and shut-down systems is given in the American Petroleum Institute Recommended Practice API RP 14c. Although intended for offshore production platforms, this standard covers many unit operations found in chemical plants and refineries. Methods for quantifying the required reliability of shut-down systems are described in Section 10.8.

If the plant safety shut-down is not rapid enough and an overpressure situation develops, the pressure relief system is activated. Pressure vessel design codes such as the ASME Boiler and Pressure Vessel Code require relief devices to be fitted on all pressure vessels. If the relief system has been properly designed and maintained, then in the event of an overpressure incident the plant contents will be vented via relief valves or bursting disks into the relief system, where liquids are recovered for treatment and vapors are sent to flare stacks or discharged to the atmosphere if it is safe to do so. The pressure relief system should allow the plant to be relieved of any source of overpressure before damage to process equipment (leaks, bursting, or explosion) can occur. Pressure relief systems are discussed in Section 10.9.

If a loss of containment does occur in a chemical plant, an emergency response is required. A small-scale loss of containment might be a leak or a spill. Leaks of liquids are usually visible and obvious, whereas leaks of vapor can be much harder to detect and require special instrumentation for monitoring. If the material that escapes from the process is flammable, the first manifestation of loss of containment might be a small or localized fire (often smoldering insulation is an early warning). Plant personnel should be trained to respond to such emergencies. Many large sites also have a dedicated emergency response staff to fight fires and clean up chemical spills. The emergency response in the process unit does not always cause the unit to be shut down, depending on the scale of the incident, but the root cause of every incident must always be determined, and any deficiency in the plant must be corrected safely before normal operations are resumed.

In the event that an incident develops into a more serious accident, the resources required will be beyond those available on the plant or site. Local community emergency response providers will be brought into the site, and injured members of the workforce and local population will need treatment at local hospitals. The local community must be able to plan for such events, and local emergency responders must be trained to cope with the hazards associated with the plant. The EPCRA ensures that the local community has access to the necessary information.

10.1.3 Intrinsic and extrinsic safety

Processes can be divided into those that are intrinsically safe and those for which the safety has to be engineered in. An intrinsically safe process is one in which safe operation is inherent in the nature of the process—a process that causes no danger, or negligible danger, under all foreseeable circumstances (all possible deviations from the design operating conditions). The term *inherently safe* is often preferred to intrinsically safe to avoid confusion with the narrower use of the term *intrinsically safe* as applied to electrical equipment (see Section 10.3.5). In the context of risk management, an inherently safe design is a design that has a very low likelihood of causing injury even in the absence of protective systems; see Section 10.8.

Clearly, the designer should always select a process that is inherently safer whenever it is practical and economic to do so; however, most chemical manufacturing processes are, to a greater or lesser extent, inherently unsafe, and dangerous situations can develop if the process conditions deviate from the design values. The safe operation of such processes depends on the design and provision of engineered safety devices and on good operating practices to prevent a dangerous situation from developing and to minimize the consequences of any incident that arises from the failure of these safeguards.

The term *engineered safety* covers the provision in the design of control systems; alarms; trips; pressure-relief devices; automatic shut-down systems; duplication of key equipment services; and firefighting equipment, sprinkler systems, and blast walls to contain any fire or explosion.

The design of inherently safer process plants is discussed by Kletz in a booklet published by the Institution of Chemical Engineers, Kletz (1984), and in Kletz and Amyotte (2010), CCPS (2012), and Chapter 32 of Mannan (2012). Kletz makes the telling point that material that is not there cannot leak out and thus cannot catch fire, explode, or poison anyone. This is a plea to keep the inventory of dangerous material to the absolute minimum required for the operation of the process. The AIChE Center for Chemical Process Safety (CCPS) has published their guidelines for inherently safer design methods in the CCPS *Guidelines for Inherently Safer Chemical Processes*, CCPS (2019), which includes a checklist for inherently safer chemical reaction process design and operation in Appendix A (available for download in the resource section on the CCPS website).

10.2 Materials hazards

In this section the special hazards of chemicals are reviewed (toxicity, flammability, and reactivity). Hazards arising from process operations will be discussed in Section 10.3.

10.2.1 Toxicity

Most of the materials used in the manufacture of chemicals are poisonous to some extent, and almost every chemical is toxic if someone is exposed to enough of it. The potential hazard will depend on the inherent toxicity of the material and the frequency and duration of any exposure.

It is usual to distinguish between the short-term (acute) effects and the long-term (chronic) effects. Acute effects normally have symptoms that develop rapidly after exposure, for example, burns to the skin after direct contact, respiratory failure, renal failure, cardiac arrest, paralysis, etc. Acute effects are usually associated with a short exposure to a high concentration of toxin (although what constitutes a "high concentration" depends on the toxicity). The chronic symptoms of poisoning develop over a long time, for example, cancer, and often persist or recur frequently. Chronic effects may occur as the result of long-term exposure to low levels of a toxin, but may also occur as a delayed response to a short-term exposure to high levels of a toxin.

Highly toxic materials that cause immediate injury, such as phosgene or chlorine, are usually classified as safety hazards, whereas materials whose effects are only apparent after long exposure at low concentrations—for instance, carcinogenic materials such as vinyl chloride—are usually classified as industrial health and hygiene hazards. The permissible limits and the precautions to be taken to ensure the limits are met will be very different for these two classes of toxic materials. Industrial hygiene is as much a matter of good operating practice and control as of good design.

The inherent toxicity of a material is measured by tests on animals. It is usually expressed as the lethal dose at which 50% of the test animals are killed, the LD_{50} (lethal dose 50) value. The dose is expressed as the quantity in milligrams of the toxic substance per kilogram of body weight of the test animal.

Some values of LD_{50} for oral ingestion by rats are given in Table 10.1. Estimates of the LD_{50} for humans are based on tests on animals. The LD_{50} measures the acute effects; it gives only a crude indication of the possible chronic effects. The LD_{50} for humans should always be taken as the lowest measured value for other mammalian species. In some cases, LD_{50} data are given for different routes of ingestion. For example, ethanol has LD_{50} values 3450 (oral, mouse), 7060 (oral, rat), and 1440 (intravenous, rat).

There is no generally accepted definition of what can be considered toxic and nontoxic.

A system of classification is given in the *Classification, Packaging and Labelling of Dangerous Substances Regulations, 1984* (United Kingdom), which is based on European Union (EU) guidelines; for example:

LD_{50}, absorbed orally in rats, mg/kg	
≤25	very toxic
25–200	toxic
200–2000	harmful

TABLE 10.1 Toxicity data

Compound	PEL (ppm)	LD_{50} (mg/kg)
Carbon monoxide	50	1807
Carbon disulfide	20	3188
Chlorine	1	239
Chlorine dioxide	0.1	292
Chloroform	50	1188
Cyclohexane	300	
Dioxane	100	4200
Ethylbenzene	100	3500
Formic acid	5	1100
Furfural	5	260
Hydrogen chloride	5	4701
Hydrogen cyanide	10	3.7
Isopropyl alcohol	400	5045
Toluene	100	5000
Xylene	100	4300

Source: OSHA.

These definitions apply only to the short-term (acute) effects. In fixing permissible limits on concentration for the long-term exposure of workers to toxic materials, the exposure time must be considered together with the inherent toxicity of the material. The "threshold limit value" (TLV) is a commonly used guide for controlling the long-term exposure of workers to contaminated air. The TLV is defined as the concentration to which it is believed the average worker could be exposed, day by day, for 8 hours a day, 5 days a week, without suffering harm. It is expressed in ppm for vapors and gases and in mg/m^3 (or $grains/ft^3$) for dusts and liquid mists. A comprehensive source of data on the toxicity of industrial materials is Sax's handbook, Lewis (2012), which also gives guidance on the interpretation and use of the data. Recommended TLV values are given by the American Conference of Government Industrial Hygienists (www.acgih.org/home). In the United States, permissible exposure limits (PEL) for known toxins are set by OSHA. Values can be found on the OSHA website at https://www.osha.gov/dsg/annotated-pels/.

Fuller details of the methods used for toxicity testing, the interpretation of the results, and their use in setting standards for industrial hygiene are given in the more specialized texts on the subject; see Carson and Mumford (1988) and Mannan (2012).

10.2.2 Flammability

The hazard caused by a flammable material depends on a number of factors:

1. The flash point of the material
2. The autoignition temperature of the material
3. The flammability limits of the material
4. The energy released in combustion

An introduction to the flammability properties of materials is given by Crowl (2012).

Flash point

The flash point is a measure of the ease of ignition of a liquid. It is the lowest temperature at which the material will ignite from an open flame. The flash point is a function of the vapor pressure and the flammability limits of the material. It is measured in standard apparatus, following standard procedures (ASTM D92 and ASTM D93). Both

open- and closed-cup apparatuses are used. Closed-cup flash points are lower than open-cup, and the type of apparatus used should be stated clearly when reporting measurements. Flash points are given in Sax's handbook, Lewis (2012). The flash points of many volatile materials are below normal ambient temperature, for example, ether −45 °C, gasoline −43 °C (open cup).

Autoignition temperature

The autoignition temperature of a substance is the temperature at which it will ignite spontaneously in air without any external source of ignition. It is an indication of the maximum temperature to which a material can be heated in air, for example, in drying operations.

Flammability limits

The flammability limits of a material are the lowest and highest concentrations in air, at normal pressure and temperature, at which a flame will propagate through the mixture. They show the range of concentration over which the material will burn in air if ignited. At very low concentrations in air a flame will not propagate, as there is insufficient fuel. Similarly, at very high concentrations a flame will not propagate due to insufficient oxidant. Flammability limits are characteristic of the particular material and differ widely for different materials. For example, hydrogen has a lower limit of 4.1 and an upper limit of 74.2% by volume, whereas for gasoline the range is only from 1.3% to 7.0%. The flammability limits for a number of materials are given in Table 10.2. The limits for a wider range of materials are given in Sax's handbook, Lewis (2012).

A flammable mixture may exist in the space above the liquid surface in a storage tank. The vapor space above highly flammable liquids is usually purged with inert gas (nitrogen), or floating-head tanks are used. In a floating-head tank a "piston" floats on top of the liquid, eliminating the vapor space.

10.2.3 Materials incompatibility

Some materials are naturally unstable and can spontaneously decompose, polymerize, or undergo other reactions. These reactions can be initiated or accelerated by promoters such as light, heat, sources of free radicals or ions or catalysts such as metal surfaces. These reactions can sometimes be retarded by adding inhibitors or diluents. Reactions of this kind are usually exothermic and if allowed to proceed will lead to a "runaway" reaction with serious consequences.

Some materials are by their nature highly reactive and will react with many other compounds at low temperatures. Examples include strong oxidizing agents such as peroxides and chlorates, strong reducing agents, strong alkalis, strong acids, and the metallic forms of alkali metals. In addition to being reactive with many other chemicals, these materials can attack the materials from which the plant is constructed.

Other groups of compounds are known to react together rapidly and exothermically. These include mixtures such as acids and bases; acids and metals; fuels and oxidants; and free radical initiators and epoxides, peroxides, or unsaturated molecules.

Another important class of incompatible materials is compounds that become more hazardous when contacted with water. For example, carbonyl sulfide (COS) and calcium sulfide (CaS) both release toxic H_2S on contact with water. Dry powders of sodium or potassium cyanide release toxic HCN in the presence of moisture. Care must be taken to prevent such materials from coming into contact with water during processing and storage. The 1985 Bhopal disaster was started by a runaway reaction involving a water-sensitive chemical.

Materials that are used to construct the process equipment and instrumentation must also be checked for compatibility with the process chemicals. This includes not only the metals or alloys from which the major vessels are built but also welding, brazing, or soldering materials; components of pumps, valves, and instruments; gaskets; seals; linings; and lubricants.

Information on incompatible materials can be found in most safety data sheets (SDSs). Wiley has published a guide to chemical incompatibilities—Pohanish and Greene (2009)—and they are also discussed in Urben (2017). The U.S. National Fire Protection Association (NFPA) also publishes standards NFPA 491 Guide to Hazardous Chemical Reactions and NFPA 49 Hazardous Chemicals Data, both of which provide data on incompatible materials.

Materials incompatibility is one of the most frequent causes of process incidents. Degradation of seals and gaskets that have become softened by solvent effects can lead to minor leaks or major loss of containment, and hence to fires, explosions, or more serious accidents. If seal or gasket leakage is identified in a process, the plant engineer should

TABLE 10.2 Flammability ranges

Material	Lower limit	Upper limit
Hydrogen	4.1	74.2
Ammonia	15.0	28.0
Hydrocyanic acid	5.6	40.0
Hydrogen sulfide	4.3	45.0
Carbon disulfide	1.3	44.0
Carbon monoxide	12.5	74.2
Methane	5.3	14.0
Ethane	3.0	12.5
Propane	2.3	9.5
Butane	1.9	8.5
Isobutane	1.8	8.4
Ethylene	3.1	32.0
Propylene	2.4	10.3
n-Butene	1.6	9.3
Isobutene	1.8	9.7
Butadiene	2.0	11.5
Benzene	1.4	7.1
Toluene	1.4	6.7
Cyclohexane	1.3	8.0
Methanol	7.3	36.0
Ethanol	4.3	19.0
Isopropanol	2.2	12.0
Formaldehyde	7.0	73.0
Acetaldehyde	4.1	57.0
Acetone	3.0	12.8
Methylethyl ketone	1.8	10.0
Dimethylamine (DEA)	2.8	184
Trimethylamine (TEA)	2.0	11.6
Gasoline	1.3	7.0
Kerosene (jet fuel)	0.7	5.6
Gas oil (diesel)	6.0	13.5

Note: Volume percentage in air at ambient conditions.

consult with the manufacturer to confirm the material is suitable for the service. If necessary, all the seals or gaskets of that material should be replaced with something more resilient to the process conditions.

10.2.4 Ionizing radiation

The radiation emitted by radioactive materials is harmful to living matter. Small quantities of radioactive isotopes are used in the process industry for various purposes—for example, in level and density-measuring instruments and for the nondestructive testing of equipment.

The use of radioactive isotopes in industry is covered by government legislation. In the United States this is under OSHA (29 CFR 1910.1096), and in Canada it is governed by the Radiation Emitting Devices Act (R.S., 1985, c. R-1). Low levels of radiation may also be present in natural minerals. Care should be taken if these radioactive materials are concentrated or accumulated in the process or dispersed into the environment.

A discussion of the particular hazards that arise in the chemical processing of nuclear fuels is outside the scope of this book.

10.2.5 Safety Data Sheets

A Safety Data Sheet (SDS) is a document summarizing the hazards and health and safety information for a chemical. In the United States, the OSHA Hazard Communication Standard (29 CFR 1910.1200) requires that chemical manufacturers must make an SDS available to employees and customers for every chemical manufactured or sold. The Canadian Hazardous Products Act (R.S., 1985, c. H-3) has the same requirement. SDSs are compliant with the UN-sponsored Globally Harmonized System (GHS) for hazard communication, as revised into the OSHA Hazard Communication Standard in 2012, and replaced the earlier MSDSs, though they contain largely the same information (Burgess, 2013).

The SDS contains the information needed to begin analyzing materials and process hazards, to understand the hazards to which the workforce is exposed, and to respond to a release of the material or other major incident where emergency response personnel may be exposed to the material.

An SDS usually contains the following sections:

1. Chemical product and company information: chemical name and grade; catalog numbers and synonyms; manufacturer's contact information, including 24-hour contact numbers
2. Composition and information on ingredients: chemical names, CAS numbers, and concentration of major components of the product
3. Hazards identification: summary of the major hazards and health effects
4. First aid measures: procedures for contact with eyes and skin or by ingestion or inhalation
5. Firefighting measures: information on firefighting, extinguishing media, flammability data, NFPA ratings
6. Accidental release measures: procedures for dealing with leaks or spills
7. Handling and storage: procedures for transfer, storage, and general use of the material
8. Exposure controls and personal protection: required engineering controls such as eyewashes, safety showers, ventilation, etc.; OSHA PEL data; required personal protective equipment
9. Physical and chemical properties
10. Stability and reactivity: conditions that cause instability, known incompatible materials, hazardous decomposition products
11. Toxicological information: acute effects, LD_{50} data, chronic effects, carcinogenicity, teratogenicity, mutagenicity
12. Ecological information: ecotoxicity data for insects and fish, other known environmental impacts
13. Disposal considerations: requirements for disposal under the Resource Conservation and Recovery Act (RCRA—see Chapter 11)
14. Transport information: shipping information required by the U.S. Department of Transport as well as other international bodies
15. Regulatory information: U.S. federal and state, European, Canadian, and international regulations listing the material; includes TSCA listing and Clean Air Act and Clean Water Act limits (see Chapter 11)
16. Additional information: date of creation and revisions, legal disclaimers

Most SDS forms are created by chemical manufacturers. They can be found in libraries, on manufacturer's websites and by contacting manufacturers or suppliers directly. Websites are available that catalogue SDS forms from multiple sources. The Canadian Centre for Occupational Health and Safety (www.msdsonline.com) also maintains an extensive database (for purchase) at their website. For legal reasons (limitation of liability), most SDS forms contain a disclaimer stating that the user should also make their own evaluation of compatibility and fitness for use. An example SDS form is given in Appendix I, available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

10.2.6 Design for materials hazards

Under OSHA hazard communication standard 29 CFR 1910.119, employers are required to carry out an assessment to evaluate the risk to health from any chemicals handled and establish what precautions are needed to protect

employees. A written record of the assessment should be kept and details made available to employees. The design engineer should consider the preventive aspects of the use of hazardous substances. Points to consider are:

1. Substitution: of the processing route with one using less hazardous material, or substitution of toxic process materials with nontoxic or less toxic materials.
2. Containment: sound design of equipment and piping to avoid leaks. For example, specifying welded joints in preference to gasketed flanged joints that are liable to leak or suffer materials incompatibility problems.
3. Prevention of releases: by process and equipment design, operating procedures, and design of disposal systems.
4. Ventilation: use open structures or provide adequate ventilation systems.
5. Disposal: provision of effective vent stacks to disperse material vented from pressure relief devices or use of vent scrubbers. Collection and treatment of sewer and run-off waters and liquids collected from relief systems.
6. Emergency equipment and procedures: automated shut-down systems, escape routes, rescue equipment, respirators, antidotes (if appropriate), safety showers, eye baths, and emergency services.

In addition, good plant operating practice would include:

1. Written instruction in the use of the hazardous substances and the risks involved.
2. Adequate training of personnel.
3. Provision of protective clothing and equipment.
4. Good housekeeping and personal hygiene.
5. Monitoring of the environment to check exposure levels. Consider the installation of permanent instruments fitted with alarms.
6. Regular medical check-ups on employees to check for the chronic effects of toxic materials.
7. Training of local emergency response personnel.

The process design engineer should always collect the SDS of every component used in the process, including solvents, acids, bases, adsorbents, etc., at as early a stage in the design as possible. The information in the SDS can be used to improve the inherent safety of the process, for example, by eliminating incompatible mixtures or substituting less hazardous chemicals as feeds, intermediates, or solvents. The SDS information can also be used to ensure that the design meets regulatory requirements on vapor recovery and other emissions.

10.3 Process hazards

In addition to the hazards caused by chemical or materials properties, hazards can arise from the conditions under which processes are carried out and the equipment that is used.

10.3.1 Pressure

Overpressure, a pressure exceeding the system design pressure, is one of the most serious hazards in chemical plant operation. If the pressure exceeds the maximum allowable working pressure of the vessel by more than the safety margin allowed in the vessel design code, then failure of the vessel can occur, usually at a joint or flange. Failure of a vessel, or the associated piping, can precipitate a sequence of events that culminate in a disaster. Overpressure occurs when mass, moles, or energy accumulate in a contained volume or space with a restricted outflow. Specific causes of overpressure are discussed in Section 10.9.1.

Pressure vessels are required to be fitted with some form of pressure-relief device, set at the maximum allowable working pressure, so that potential overpressure is relieved in a controlled manner (ASME Boiler and Pressure Vessel Code, Section VIII Division 1, Part UG-125). See Section 10.9 for a more detailed discussion of pressure relief.

Process equipment must also be protected from underpressure (vacuum), as this places compressive stresses on vessel walls that can lead to failure by bucking. Design for underpressure is discussed in Section 10.9.6.

The factors to be considered in the design of relief systems are set out in a comprehensive paper by Parkinson (1979) and by Moore (1984). More extensive references, including design codes and standards and relief system design software, are given in Section 10.9.

10.3.2 Temperature deviations

Excessively high temperature, over and above that for which the equipment was designed, can cause structural failure and initiate a disaster. High temperatures can arise from loss of control of reactors and heaters and, externally, from open fires. In the design of processes where high temperatures are a hazard, protection against high temperatures is provided by:

1. Provision of high-temperature alarms and interlocks to shut down reactor feeds, or heating systems, if the temperature exceeds critical limits.
2. Use of additional temperature detectors to provide highly localized and redundant temperature monitoring. These include detectors on the wall of the vessel ("skin thermocouples") as well as in thermowells exposed to the process fluids. In some cases, temperature-sensitive paint that changes color above a certain threshold is used on the outside of the vessel.
3. Provision of emergency cooling systems for reactors where heat continues to be generated after shut-down, for instance, in some polymerization systems.
4. Provision of quench systems for emergency shut-down, designed to flood the equipment with a cold, inert material.
5. Structural design of equipment to withstand the worst possible temperature excursion.
6. The selection of inherently safe heating systems for hazardous materials.

Steam and other vapor heating systems are inherently safer than fired heat and electric heat, as the temperature cannot exceed the saturation temperature at the supply pressure if the vapor is de-superheated and the supply line has a relief system that prevents it from becoming overpressurized. Other heating systems rely on control of the heating rate to limit the maximum process temperature. Electrical heating systems can be particularly hazardous, because the heating rate is proportional to the resistance of the heating element, which increases with temperature.

Very low temperatures can also be hazardous. Low temperatures can be caused by ambient conditions, operation of cryogenic processes, expansion of gases and vapors, flashing of liquids (autorefrigeration), and endothermic reactions. Low temperatures can cause embrittlement and stress cracking in metals. At very low temperatures some metals undergo microstructural transformations that cause substantial changes in density (for example, brass). When water freezes in a confined volume, the increase in specific volume can cause pipes or vessels to crack. Minimum design metal temperatures are specified in pressure vessel design (see Chapter 14).

10.3.3 Noise

Excessive noise is a hazard to health and safety. Long exposure to high noise levels can cause permanent damage to hearing. At lower levels, noise is a distraction and causes fatigue. Regulations on noise are set by OSHA (29 CFR 1910.95, 2007).

The unit of sound measurement is the decibel, defined by the expression:

$$\text{Sound level} = 20 \log_{10}\left[\frac{\text{RMS sound pressure (Pa)}}{2 \times 10^{-5}}\right], \text{dB} \tag{10.1}$$

The subjective effect of sound depends on frequency as well as intensity.

Industrial sound meters include a filter network to give the meter a response that corresponds roughly to that of the human ear. This is termed the *"A" weighting network*, and the readings are reported as dB(A). Permanent damage to hearing can be caused at sound levels above about 85 dB(A), and it is normal practice to provide ear protection in areas where the level is above 80 dB(A).

Excessive plant noise can lead to complaints from neighboring factories and local residents. Due attention should be given to noise levels when specifying, and when laying out, equipment that is likely to be excessively noisy, such as compressors, fans, burners, and steam relief valves. This equipment should not be placed near the control room.

Several books are available on the general subject of industrial noise control—Bies and Hansen (2009)—and on noise control in the process industries—Cheremisinoff (1996) and IMechE (1993).

10.3.4 Loss of containment

The primary means for protecting employees and the public from exposure to toxic chemicals is the plant itself. Loss of containment can occur due to:

1. Pressure relief events.
2. Operator errors such as leaving a sample point open or dripping.
3. Poor maintenance procedures, including failure to isolate, drain, and purge properly before maintenance, leading to release when the equipment is opened, or failure to reconnect items properly and close drain valves when maintenance is complete.
4. Leaks from degraded equipment, including damaged seals, gaskets, and packings and corroded or eroded vessels and pipes.
5. Emissions from solid-handling operations (dust).
6. Internal equipment leaks (particularly in heat exchanger tubesheets) that allow utility services such as cooling water to become contaminated with process chemicals.
7. Spills from drum or tanker loading and emptying.

Frequent loss-of-containment incidents are usually an indication that a plant has been poorly maintained and are a leading indicator of major incidents.

If the potential impact of a loss of containment is high, then the design engineer should provide a means of containment or mitigation. These means might include:

1. Secondary containment (bunding) to prevent run-off, but note that this can create a worse hazard if the chemicals are flammable and easily ignited.
2. Contained drainage and sewer systems to collect run-off and rainwater for waste treatment.
3. Use of concrete foundations to protect groundwater.
4. Containment of the plant inside a building with ventilation and vent scrubbers (used for hazardous dusts and highly toxic compounds).

10.3.5 Fires and ignition sources

A fire occurs whenever sufficient amounts of fuel and oxidant are mixed and contacted with an ignition source. If a fuel is above its autoignition temperature, then ignition can occur spontaneously in air. Though precautions are normally taken to eliminate sources of ignition on chemical plants, it is best to work on the principle that a leak of flammable material will ultimately find an ignition source. Guidelines for the control of ignition sources are given in section 7.9 of NFPA 30.

Electrical equipment

The sparking of electrical equipment, such as motors, is a major potential source of ignition, and flameproof equipment is normally specified. Electrically operated instruments, controllers, and computer systems are also potential sources of ignition of flammable mixtures.

The use of electrical equipment in hazardous areas is covered by the National Electrical Code (NFPA standard 70), NFPA standards 496 and 497, and OSHA standard 29 CFR 1910.307. The American Petroleum Institute Recommended Practices API RP 500 and API RP 505 should also be consulted.

Articles 500 and 505 of the National Electrical Code (NFPA 70) define classified areas in which flammable materials may be present at high enough concentrations to be ignitable. In a Class I location, the ignitable material is a gas or vapor. Class I locations are further divided into either divisions or zones as follows:

Class I, Division 1: locations in which ignitable concentrations of flammable gas or vapor can exist under normal operating conditions; or can exist frequently because of repair, maintenance or leakage; or can be released during breakdown or faulty operation of equipment that might also cause simultaneous failure of electrical equipment such that the electrical equipment could become a source of ignition.

Class I, Division 2: locations in which flammable gases, vapors, or volatile liquids are processed but are normally contained within closed systems; or ignitable concentrations are normally prevented by forced ventilation; or the location is adjacent to a Class I, Division 1 location and an ignitable concentration of gas or vapor might occasionally be communicated to it.

Class I, Zone 0: locations in which ignitable concentrations of vapor or gas are present continuously or for long periods.

Class I, Zone 1: locations where ignitable concentrations of flammable gas or vapor are likely to exist under normal operating conditions; or may exist frequently because of repair, maintenance, or leakage; or could be released by equipment breakdown or faulty operation that could simultaneously cause failure of the electrical

equipment in such a way that the electrical equipment could act as a source of ignition; or is adjacent to a Class I, Zone 0 location from which ignitable concentrations of flammable gas or vapor could be communicated.
Class I, Zone 2: locations where ignitable concentrations of flammable gas or vapor are not likely to exist in normal operation, and if they do occur will exist only for short periods; or flammable gases, vapors, or liquids are processed but are normally contained within closed systems; or ignitable concentrations are normally prevented by forced ventilation; or the location is adjacent to a Class I, Zone 1 location and an ignitable concentration of gas or vapor might occasionally be communicated to it.

Guidance on how to classify a location is given in the standards NFPA 30, NFPA 497, API RP 500, and API RP 505.

Various protection techniques can be used to prevent electrical equipment from becoming an ignition source. Explosion-proof enclosures, pressurized and purged equipment, and intrinsically safe circuits can be used in Division 1 and Division 2 locations. Nonsparking equipment can be used in Division 2 locations. Details of the types of equipment permitted in each classified location are given in NFPA 70.

It is also important that electrical equipment in hazardous areas be properly maintained, particularly in older plants. Guidelines for maintenance of electrical equipment are given in standard NFPA 70B.

The standards should be consulted for the full specification before selecting equipment for use in classified locations.

The design and specification of intrinsically safe control equipment and systems is discussed by MacMillan (1998) and Cooper and Jones (1993). Purged and pressurized enclosures for electrical equipment are described in NFPA 496.

Static electricity

The movement of any nonconducting material, powder, liquid, or gas can generate static electricity, producing sparks. Precautions must be taken to ensure that all piping is properly earthed (grounded) and that electrical continuity is maintained around flanges. Escaping steam, or other vapors and gases, can generate a static charge. Gases escaping from a ruptured vessel can self-ignite from a static spark. For a review of the dangers of static electricity in the process industries, see the article by Napier and Russell (1974) and the books by Pratt (1997) and Britton (1999). Protection against static electricity, lightning, and stray currents is discussed in API RP 2003. The NFPA standard NFPA 77 is the national standard on static electricity protection in the United States.

Process flames

Open flames from process furnaces, incinerators, and flare stacks are obvious sources of ignition and must be sited well away from plants containing flammable materials.

Miscellaneous sources

It is the usual practice in plants handling flammable materials to control the entry to the site of obvious sources of ignition, such as matches, cigarette lighters, and battery-operated equipment. The use of portable electrical equipment, welding, cutting, and spark-producing tools and the movement of gasoline engine vehicles would also be subject to strict control. Exhaust gases from diesel engines are also a potential source of ignition.

Flame traps

Flame arresters are fitted in the vent lines of equipment that contains flammable material to prevent the propagation of flame through the vents. Various types of proprietary flame arresters are used. In general, they work on the principle of providing a heat sink, usually expanded metal grids or plates, to dissipate the heat of the flame. Flame arrestors and their applications are discussed by Rogowski (1980), Howard (1992), Mendoza et al. (1998), API RP 2210, and BS EN ISO 16852.

Traps should also be installed in plant ditches to prevent the spread of flame. These are normally liquid U-legs, which block the spread of a flame along ditches.

Fire protection

Recommendations on the fire precautions to be taken in the design of chemical plants are given in the standards NFPA 30, API RP 2001, and API RP 2218. Legal requirements for fire protection are given in the OSHA standard 29 CFR 1910, subpart L. The relevant international standard is BS EN ISO 19353.

To protect against structural failure, water deluge systems are usually installed to keep vessels and structural steelwork cool in a fire. Water-mist fire protection systems are described in NFPA 750 and API RP 2030. The lower sections of structural steel columns are often lagged with concrete or other suitable materials.

Plants that handle flammable liquids are usually designed to have slightly sloping ground or use drainage ditches or trenches to control run-off so that pools do not form. Drainage ditches and slopes should always direct flow away from sources of ignition.

10.3.6 Explosions

An explosion is the sudden, catastrophic release of energy, causing a pressure wave (blast wave). An explosion can occur without fire, such as the failure through overpressure of a steam boiler or an air receiver. A good general introduction to explosions is given by Crowl (2003).

When discussing the explosion of a flammable mixture, it is necessary to distinguish between detonation and deflagration. If a mixture detonates, the reaction zone propagates at a supersonic velocity (above approximately 300 m/s) and the principal heating mechanism in the mixture is shock compression. The pressure wave in a detonation can be up to 20 bar. In a deflagration, the combustion process is the same as in the normal burning of a gas mixture, the combustion zone propagates at a subsonic velocity, and the pressure build-up is slow and usually less than 10 bar. Whether detonation or deflagration occurs in a gas–air mixture depends on a number of factors, including the concentration of the mixture and the source of ignition. Unless confined or ignited by a high-intensity source (a detonator), most materials will not detonate; however, the pressure wave (blast wave) caused by a deflagration can still cause considerable damage. In a confined space, such as a pipe or inside a building, a deflagration can propagate into a detonation.

Certain materials—for example, acetylene and many peroxides—can decompose explosively in the absence of oxygen; such materials are particularly hazardous.

Confined vapor cloud explosion (CVCE)

A relatively small amount of flammable material—a few kilograms—can lead to an explosion when released into the confined space of a building.

Unconfined vapor cloud explosion (UCVCE)

This type of explosion results from the release of a considerable quantity of flammable gas, or vapor, into the atmosphere and its subsequent ignition. Such an explosion can cause extensive damage, such as occurred at Flixborough, HMSO (1975) and BP Texas City, CSHIB (2005). Unconfined vapor explosions are discussed by Munday (1976) and Gugan (1979).

Boiling liquid expanding vapor explosion (BLEVE)

BLEVEs occur when there is a sudden release of vapor containing liquid droplets due to the failure of a vessel. A serious incident involving the failure of a liquefied petroleum gas (LPG) storage sphere occurred at Feyzin, France, in 1966, when the tank was heated by an external fire fueled by a leak from the tank; see Mannan (2012) and Marshall (1987).

Dust explosions

Finely divided combustible solids, if intimately mixed with air, can explode. Several disastrous explosions have occurred in grain silos and sugar factories.

Dust explosions usually occur in two stages: a primary explosion that disturbs deposited dust, followed by the second, more severe, explosion of the dust thrown into the atmosphere. Any finely divided combustible solid is a potential explosion hazard. Particular care must be taken in the design of dryers, conveyors, cyclones, and storage hoppers for polymers and other combustible products or intermediates. The extensive literature on the hazard and control of dust explosions should be consulted before designing powder handling systems: Field (1982), Cross and Farrer (1982), Barton (2001), Eckhoff (2003), NFPA 61, NFPA 654, NFPA 664, and BS EN 1127.

Explosivity properties

Information on explosive materials is given in the standards NFPA 495, NFPA 491, and BS EN 1839. *Sax's Handbook of Hazardous Materials* (Lewis, 2012) is also a good general reference.

The expansion factor is defined as the molar density of the reagents divided by the molar density of the products in an explosive mixture. The expansion factor is a measure of the increase in volume resulting from combustion. The maximum value of the expansion factor is for adiabatic combustion.

The flame speed is the rate of propagation of a flame front through a flammable mixture with respect to a fixed observer. Materials such as hydrogen and acetylene that have high flame speeds are more prone to detonation.

Values of these properties, autoignition temperature and adiabatic flame temperature are given for hydrogen and some hydrocarbons in Table 10.3, which is based on data from Drysdale (2011).

Design implications

The usual approach in design is to prevent explosions from occurring, for example, by not allowing flammable mixtures to form in the process. If internal explosion is a possibility, then it must be considered as a pressure relief scenario and the pressure relief devices must be sized to prevent detonation. This will usually require the use of large bursting disks; see Section 10.9. Flame arrestors should also be specified on process piping to prevent a deflagration event from propagating into a detonation. Particular care should be taken when designing plants that contain both pressurized fuels and pressurized oxidants. General guidelines on explosion protection are given in NFPA 69 and NFPA 68; see also the European standards BS EN 1127, BS EN 14460, and BS EN 60079 and the references listed in Section 10.3.5. Explosion suppression and venting systems are discussed in BS EN 14373, BS EN 14797, and BS EN 14994. Specific guidelines for various sectors of the process industries are given in other standards, such as offshore production installations (BS EN ISO 13702), agricultural and food processing plants (NFPA 61), wood processing and woodworking facilities (NFPA 664), and plants handling sulfur (NFPA 655).

10.3.7 Human error

The intervention of well-trained process operators is a vital layer in process safety, as it is usually the last opportunity to restore the process to a safe condition before an emergency shut-down or incident occurs (see Fig. 10.1).

Even with computer control of basic plant regulatory control systems and a capable, experienced, and well-trained staff, there is always a possibility of human error. Kletz et al. (1995) describe incidents that have occurred due to human errors in control system design, installation, and operation. The likelihood of operator error is substantially increased if operating procedures are not clearly documented and followed or if there are lapses in training and supervision. Kletz (1999) has suggested the following failure probabilities:

TABLE 10.3 Explosivity properties

Fuel	Formula	Maximum flame speed (m/s)	Adiabatic flame temperature (K)	Expansion factor	Autoignition temperature (°C)
Hydrogen	H_2	22.1	2318	6.9	400
Methane	CH_4	2.8	2148	7.5	601
Ethane	C_2H_6	3.4	2168	7.7	515
Propane	C_3H_8	3.3	2198	7.9	450
n-Butane	C_4H_{10}	3.3	2168	7.9	405
Pentane	C_5H_{12}	3.4	2232	8.1	260
Hexane	C_6H_{14}	3.4	2221	8.1	225
Acetylene	C_2H_2	14.8	2598	8.7	305
Ethylene	C_2H_4	6.5	2248	7.8	490
Propylene	C_3H_6	3.7	2208	7.8	460
Benzene	C_6H_6	5	2287	8.1	560
Cyclohexane	C_6H_{12}	4.2	2232	8.1	245

Adapted from Drysdale (2011).

Action required	Probability of failure
A valve to be closed directly below an alarm	0.001
Simple action in a quiet environment	0.01
Simple action in a distracting environment	0.1
Complex and rapid action required	1.0

The Chemical Safety and Hazard Investigation Board (CSHIB) preliminary report on their investigation of the explosion at the BP Texas City refinery on March 23, 2005, in which 15 people were killed and over 170 were injured, describes multiple failures in supervision, operating procedures, and training that contributed to the accident (CSHIB, 2005). One of these was holding a safety training meeting in the control room while the operators were trying to start up the plant.

10.4 Analysis of product and process safety

The analysis of health, safety, and environmental (HS&E) impact of technology is so important that it is carried out at every stage of a project, using the project technical information as it becomes available. As more design detail is developed, more quantitative methods can be used for analyzing safety and environmental impact.

Table 10.4 shows typical steps in the evolution of a new product or process from initial concept to manufacture. In the early stages of process development, the detail of the process has not been established, but qualitative

TABLE 10.4 Health, safety, and environmental impact analysis during the evolution of a project

Stage	Information available	HS&E analysis methods
Research concept	Chemistry	SDS review
	SDS information	major hazard review
Conceptual design	Process flow diagram	Process FMEA/HAZAN
	Equipment list	Pollution prevention analysis
	Vessel designs	Preliminary operating procedures
Reactor models		
Preliminary design	P&I diagrams	HAZOP
	Process control scheme	Emergency procedures
	Metallurgy	Safety indices
	Detailed mass and energy balance	Safety checklists
	Hydraulics	Effluent summary
	Offsites	
Detailed design	Mechanical designs	Quantitative risk analysis
engineering	Instrument specs	Fault tree analysis
	Vendor details	
	Plot plans	
Procurement, construction	Piping isometrics	As built HAZOP
	As-built specs	Operator training
Operation	Commissioning log	Ongoing training
	Operations log	Change management procedures
	Maintenance log	Revised operating procedures

assessments of major hazards can be made by collecting information from the SDS forms for the chemicals involved. Once a conceptual flow scheme has been developed, semi-quantitative methods such as failure mode and effects analysis (FMEA—see Section 10.5) and systematic procedures for identifying hazards such as HAZAN can be applied. An initial pollution prevention analysis can be made if the major process effluents are known. Some companies also calculate safety indices at this stage to give a semi-quantitative comparison of the safety of the new process compared with existing processes (Section 10.6). When the process P&I diagram has been established and a full mass and energy balance has been completed, a full hazard and operability study (HAZOP—see Section 10.7) can be carried out and the operating and emergency procedures can be updated. Safety checklists (Section 10.4.1) are often completed at this stage and then updated and amended at subsequent stages. During detailed design and procurement, vendor information on instrument reliability becomes available. This information can be used to make a more quantitative analysis of likely failure rates, and hence determine whether duplicate or backup systems are needed (Section 10.8). When the plant begins operation, any changes or modifications made during commissioning or in operation must also go through a detailed hazard analysis.

In the United States, the OSHA standard 29 CFR 1910.119 *Process Safety Management of Highly Hazardous Chemicals* requires that a hazard analysis must be carried out for any process involving certain listed chemicals (see Appendix A of the standard) or involving more than 10,000 lb (4535.9 kg) of flammable gas or liquid. Employers must involve employees in the hazard analysis, and it must be made available to employees and updated at least every 5 years. Employees and contractors must be trained in safe work practices associated with the identified process hazards. Full details of these and other legal requirements, as well as descriptions of the information that must be included in the analysis, can be found in the standard. The most recent version of this standard and all other OSHA regulations are available at www.osha.gov. The regulations do not specify the method of hazard analysis that must be used, and most employers use several or all of the methods listed in the following sections, increasing the complexity of the analysis as more information is developed during the course of the project.

When the product that will be produced by the plant is a food, vitamin, cosmetic, medical implant, or human or veterinary drug additional safety analysis must be carried out to comply with regulations set by the Food and Drug Administration (FDA). The FDA requires that plants that come under its jurisdiction must follow Current Good Manufacturing Practice (CGMP) regulations. Additional documentation of the design and operation of such plants is required, and these documents are subject to inspection and certification by the FDA. Details of FDA regulations can be found in the FDA Compliance Policy Guides, which are available at www.fda.gov. GMP guidelines are addressed in more detail in the discussion of bioreactor quality control in Section 15.9.8.

Overviews of the different methods used for safety analysis are given in Crowl and Louvar (2019), Mannan (2012), CCPS (2008), and BS EN ISO 17776 (2000).

10.4.1 Safety checklists

Checklists are useful aids to memory. A checklist that has been drawn up by experienced engineers can be a useful guide for the less experienced; however, too great a reliance should never be put on the use of checklists to the exclusion of other considerations and techniques. No checklist can be completely comprehensive, covering all the factors to be considered for any particular process or operation.

A short safety checklist, covering the main items that should be considered in process design, is given here. More detailed checklists are given by Carson and Mumford (1988) and Wells (1980). Balemans (1974) gives a comprehensive list of guidelines for the safe design of chemical plants drawn up in the form of a checklist. A loss prevention checklist is included in *Dow's Fire and Explosion Index Hazard Classification Guide* (Dow, 1994).

Design safety checklist

Materials

a. flash point
b. flammability range
c. autoignition temperature
d. composition
e. stability (shock sensitive?)
f. toxicity, TLV
g. corrosion
h. physical properties (unusual?)
i. heat of combustion/reaction

Process

1. Reactors
   a. exothermic − heat of reaction
   b. temperature control − emergency systems
   c. side reactions − dangerous?
   d. effect of contamination
   e. effect of unusual concentrations (including catalyst)
   f. corrosion
2. Pressure systems
   a. need?
   b. design to current codes
   c. materials of construction − adequate?
   d. pressure relief − adequate?
   e. safe venting systems
   f. flame arresters

Control systems

a. fail safe
b. backup power supplies
c. high/low alarms and trips on critical variables
   i. temperature
   ii. pressure
   iii. flow
   iv. level
   v. composition
d. backup/duplicate systems on critical variables
e. remote operation of valves
f. block valves on critical lines
g. excess-flow valves
h. interlock systems to prevent misoperation
i. automatic shut-down systems

Storage

a. limit quantity
b. inert purging/blanketing
c. floating roof tanks
d. dykeing
e. loading/unloading facilities − safety
f. earthing
g. ignition sources − vehicles

General

a. inert purging systems needed
b. compliance with electrical codes
c. adequate lighting
d. lightning protection
e. sewers and drains adequate, flame traps
f. dust-explosion hazards
g. buildup of dangerous impurities − purges
h. plant layout
   i. separation of units
   ii. access
   iii. siting of control rooms and offices
   iv. services
i. safety showers, eye baths

Fire protection

a. emergency water supplies
b. fire mains and hydrants
c. foam systems
d. sprinklers and deluge systems
e. insulation and protection of structures
f. access to buildings
g. firefighting equipment

The checklist is intended to promote thought and to raise questions such as: Is it needed? What are the alternatives? Has provision been made for…? Has it been checked for…? Has it been provided?

10.5 Failure mode effect analysis

Failure mode and effects analysis (FMEA) is a method originally developed in manufacturing, which is used to determine the relative importance of different component failures within an overall system or product. It can be applied to analysis of chemical plant safety (OSHA 29 CFR 1910.119), as well as to design of products and even business plans and commercial projects. The method is semi-quantitative. It assigns numerical rankings to different failure modes based on the (qualitative) perceptions of the participants. Different groups or individuals will not necessarily reach the same conclusions, so the method is best used in the early stages of design as a means of brainstorming for safety issues. More rigorous methods such as HAZAN and HAZOP should be applied when more design details are available.

10.5.1 FMEA procedure

An FMEA should ideally be carried out as a group brainstorming exercise. The group should include a diverse set of experts. When an FMEA is used for process safety analysis, these should include:

1. An expert on process chemistry
2. An expert on process equipment
3. An expert on process control
4. An expert on process operations
5. An expert on safety analysis
6. The process design engineer

The analysis then proceeds as follows:

1. The group begins by reviewing the process and defining a set of process steps or key inputs.
2. For each step or input, they then brainstorm for failure modes (i.e., ways in which the step or input might not perform its desired function).
3. For each failure mode, the group brainstorms possible consequences. There may be multiple consequences for a given failure mode.
4. For each failure mode (and consequences) the group lists possible causes. Once again, several causes may trigger the same failure mode.
5. For each cause, the team lists the systems *that are currently in place* to prevent the cause from happening or allow the cause to be detected in time for operators to respond before the failure mode occurs. At this step, it is very important that the team considers the design as it currently exists. They must not assume that something will be added later to take care of any identified problem.
6. Once the brainstorming phase is completed (usually after several sessions), the team reviews the list of consequences and assigns each of them a "severity" number (SEV). The severity is a measure of the impact of the consequence. Different scales can be used for severity, as discussed in Section 10.5.2.
7. The team then assigns a "likelihood of occurrence" number (OCC) to each of the causes. The occurrence number is a measure of either the probability or frequency of the cause occurring.
8. For each of the current control methods or systems, the team assigns a "detection" number (DET) that rates the probability that the existing systems will prevent the cause or failure mode from happening or detect the cause and allow an operator response before the failure mode occurs.

9. The three numbers, SEV, OCC, and DET, are multiplied together to give an overall risk probability number (RPN).
10. Based on the RPN values, actions are assigned to each item in the FMEA. Low RPN items may require no action, whereas high RPN issues may require major changes to the process design and instrumentation.

An FMEA should always be associated with a particular revision of a design. Whenever a new revision is released, the FMEA should be updated.

10.5.2 FMEA rating scales

The numbers assigned to the FMEA SEV, OCC, and DET parameters are only a qualitative indication of the probability or impact. Because of this (and to reduce the time spent arguing over whether an item deserves a 4 or a 5 rating) most experienced practitioners use a 1, 4, 7, 10 scale to increase the granularity of the responses.

It is important that the team agree on the meaning of each rating in the context of each of the FMEA parameters before starting to assign ratings. A suggested rating scale is given in Table 10.5, but other scales may be more appropriate in other cases.

It should be noted that the DET scale is inverse to the OCC scale. A high value of the DET number corresponds to a low probability of detection, whereas a high value of the OCC number corresponds to a high probability of occurrence.

When assigning ratings to the different FMEA parameters, it is good practice to attempt to reach a consensus within the team. If no consensus can be developed (usually between a pair of values), then the best practice is to choose the higher value of the pair.

10.5.3 Interpretation of FMEA scores

Once the RPN values have been calculated, the list should be ranked by RPN and should be checked for consistency. This is particularly necessary when the FMEA has been completed during several sessions. FMEA is essentially a qualitative method, and the rankings based on RPN are, at best, only an indication of the team's assessment of the relative risk of the different failure modes. The team should not be overly concerned with the relative ranking of two issues as long as both are ranked appropriately high or low in the overall list.

Every item in the list should be reviewed to determine what follow-up action is required. If a 1, 4, 7, 10 scale is used, then specific actions leading to changes in design or operating procedures are usually required for every item with an RPN score greater than 100. This ensures that any item that scores 7 or 10 in one rating leads to an action unless it scores 1 in one of the other ratings.

Because FMEA is a qualitative method, it is difficult to draw comparisons between FMEA studies of different processes. If a team studying process A identifies 70 items in an FMEA, whereas a team studying process B identifies 200 items, then either process B has more associated risks or the team assigned to process B made a more thorough analysis. A short list of FMEA items (fewer than 50) usually indicates an incomplete analysis rather than a safe process.

TABLE 10.5 Suggested rating scale for FMEA

Rating	SEV	OCC	DET
1	Effect is insignificant	Failure is very unlikely	Current safeguards will always prevent failure mode
4	Minor disruption, possible loss of production	Occasional failure possible	High probability that current safeguard will detect or prevent
7	Major disruption, possible damage to local equipment	Infrequent failure is likely	Low probability that current safeguard will detect or prevent
10	Severe disruption, major damage to plant, possible injury to personnel	Failure is very likely or frequent	No current method of detection

10.5.4 Tools for FMEA

Failure mode and effects analysis (FMEA) is easily carried out using spreadsheets. A Microsoft Excel template is available in Appendix G in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793. Additional information on FMEA is given by Birolini (2017), Dodson and Nolan (1999), and Stamatis (2003, 2019).

10.6 Safety indices

Some companies make use of safety indices as a tool for assessing the relative risk of a new process or plant. The most widely used safety index is the Dow Fire and Explosion Index, developed by the Dow Chemical Company and published by the American Institute of Chemical Engineers (Dow, 1994) (www.aiche.org). A numerical "fire and explosion index" (F&EI) is calculated, based on the nature of the process and the properties of the process materials. The larger the value of the F&EI, the more hazardous the process (Table 10.6).

To assess the potential hazard of a new plant, the index can be calculated after the piping and instrumentation and equipment layout diagrams have been prepared. In earlier versions of the guide, the index was then used to determine what preventive and protection measures were needed; see Dow (1973). In the current version, the preventive and protection measures that have been incorporated in the plant design to reduce the hazard are taken into account when assessing the potential loss in the form of loss control credit factors.

It is worthwhile to estimate the F&EI at an early stage in the process design, as it will indicate whether alternative, less hazardous process routes should be considered.

Only a brief outline of the method used to calculate the Dow F&EI will be given in this section. The full guide should be studied before applying the technique to a particular process. Judgment, based on experience with similar processes, is needed to determine the magnitude of the various factors used in the calculation of the index and the loss control credit factors.

10.6.1 Calculation of the Dow F&EI

The procedure for calculating the index and the potential loss is set out in Fig. 10.2.

The first step is to identify the units that would have the greatest impact on the magnitude of any fire or explosion. The index is calculated for each of these units.

The basis of the F&EI is a *material factor* (MF). The MF is then multiplied by a *unit hazard factor*, F_3, to determine the F&EI for the process unit. The unit hazard factor is the product of two factors that take account of the hazards inherent in the operation of the particular process unit: the general and special process hazards (Fig. 10.3).

Material factor

The material factor is a measure of the intrinsic rate of energy release from the burning, explosion, or other chemical reaction of the material. Values for the MF for over 300 of the most commonly used substances are given in the guide. The guide also includes a procedure for calculating the MF for substances not listed: from knowledge of the flash points (for dusts, dust explosion tests) and a reactivity value, N_r. The reactivity value is a qualitative description of the reactivity of the substance and ranges from 0 for stable substances to 4 for substances that are capable of unconfined detonation. Some typical material factors are given in Table 10.7.

In calculating the F&EI for a unit, the value for the material with the highest MF, which is present in significant quantities, is used.

TABLE 10.6 Assessment of hazards

Fire and Explosion Index range	Degree of hazard
1–60	Light
61–96	Moderate
97–127	Intermediate
128–158	Heavy
>159	Severe

Adapted from Dow (1994).

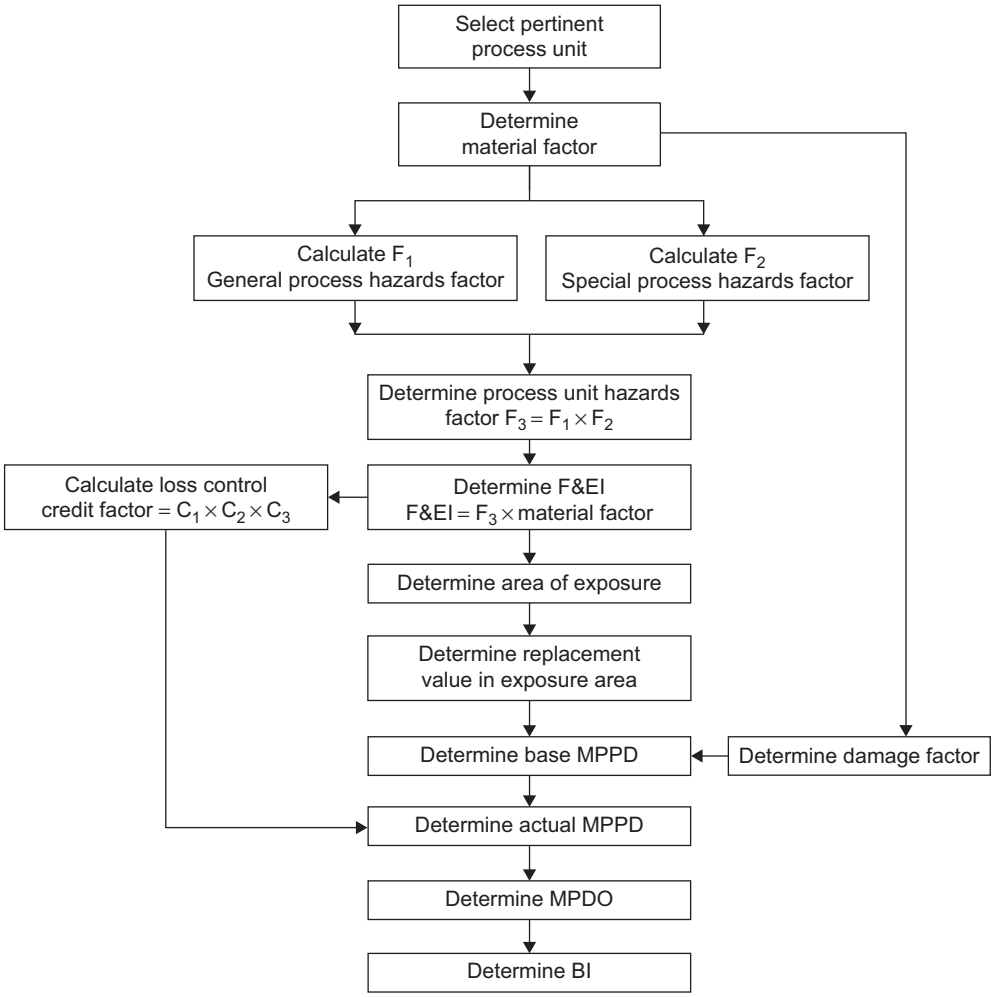


FIG. 10.2 Procedure for calculating the Fire and Explosion Index and other risk analysis information. *From Dow [1994] reproduced by permission of the American Institute of Chemical Engineers. © 1994 AIChE. All rights reserved.*

General process hazards

The general process hazards are factors that play a primary role in determining the magnitude of the loss after an incident.

Six factors are listed on the calculation form (see Fig. 10.3).

A. *Exothermic chemical reactions*: The penalty varies from 0.3 for a mild exotherm, such as hydrogenation, to 1.25 for a particularly sensitive exotherm, such as nitration.
B. *Endothermic processes*: A penalty of 0.2 is applied to reactors only. It is increased to 0.4 if the reactor is heated by the combustion of a fuel.
C. *Materials handling and transfer*: This penalty takes account of the hazard involved in the handling, transfer, and warehousing of the material.
D. *Enclosed or indoor process units*: Accounts for the additional hazard where ventilation is restricted.
E. *Access of emergency equipment*: Areas not having adequate access are penalized. Minimum requirement is access from two sides.
F. *Drainage and spill control*: Penalizes design conditions that would cause large spills of flammable material adjacent to process equipment, such as inadequate design of drainage.

Special process hazards

The special process hazards are factors that are known from experience to contribute to the probability of an incident involving loss.

Twelve factors are listed on the calculation form (see Fig. 10.3).

FIRE & EXPLOSION INDEX

AREA/COUNTRY	DIVISION	LOCATION	DATE
SITE	MANUFACTURING UNIT	PROCESS UNIT	
PREPARED BY:	APPROVED BY:(Superintendent)	BUILDING	
REVIEWED BY:(Management)	REVIEWED BY:(Technology Center)	REVIEWED BY:(Safety & Loss Prevention)	
MATERIALS IN PROCESS UNIT			
STATE OF OPERATION — DESIGN — START UP — NORMAL OPERATION — SHUTDOWN	BASIC MATERIAL(S) FOR MATERIAL FACTOR		
MATERIAL FACTOR (See Table 1 or Appendices A or B) Note requirements when unit temperature over 140 °F (60 °C)			

1. General Process Hazards	Penalty Factor Range	Penalty Factor Used(1)
Base Factor	1.00	1.00
A. Exothermic Chemical Reactions	0.30 to 1.25	
B. Endothermic Processes	0.20 to 0.40	
C. Material Handling and Transfer	0.25 to 1.05	
D. Enclosed or Indoor Process Units	0.25 to 0.90	
E. Access	0.20 to 0.35	
F. Drainage and Spill Control _____ gal or cu.m.	0.25 to 0.50	
General Process Hazards Factor (F_1)		
2. Special Process Hazards		
Base Factor	1.00	1.00
A. Toxic Material(s)	0.20 to 0.80	
B. Sub-Atmospheric Pressure (< 500 mm Hg)	0.50	
C. Operation In or Near Flammable Range ___ Inerted ___ Not Inerted		
1. Tank Farms Storage Flammable Liquids	0.50	
2. Process Upset or Purge Failure	0.30	
3. Always in Flammable Range	0.80	
D. Dust Explosion (See Table 3)	0.25 to 2.00	
E. Pressure (See Figure 2) Operating Pressure _____ psig or kPa gauge; Relief Setting _____ psig or kPa gauge		
F. Low Temperature	0.20 to 0.30	
G. Quantity of Flammable/Unstable Material: Quantity _____ lb or kg; H_C = _____ BTU/lb or kcal/kg		
1. Liquids or Gases in Process (See Figure 3)		
2. Liquids or Gases in Storage (See Figure 4)		
3. Combustible Solids in Storage, Dust in Process (See Figure 5)		
H. Corrosion and Erosion	0.10 to 0.75	
I. Leakage – Joints and Packing	0.10 to 1.50	
J. Use of Fired Equipment (See Figure 6)		
K. Hot Oil Heat Exchange System (See Table 5)	0.15 to 1.15	
L. Rotating Equipment	0.50	
Special Process Hazards Factor (F_2)		
Process Unit Hazards Factor (F_1 x F_2) = F_3		
Fire and Explosion Index (F_3 x MF = F&EI)		

(1) For no penalty use 0.00.

(a)

FIG. 10.3 Dow Fire and Explosion Index calculation form. Note: The figure numbers refer to the Dow guide. Gallons are U.S. gallons. Note: 1 m^3 = 264.2 U.S. gal; 1 kN/m^2 = 0.145 psi; 1 kg = 2.2 lb; 1 kJ/Kg = 0.43 BTU/lb.

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TABLE 10.7 Some typical material factors

	MF	Flash point °C	Heat of combustion MJ/kg
Acetaldehyde	24	−39	24.4
Acetone	16	−20	28.6
Acetylene	40	gas	48.2
Ammonia	4	gas	18.6
Benzene	16	−11	40.2
Butane	21	gas	45.8
Chlorine	1	–	0.0
Cyclohexane	16	−20	43.5
Ethyl alcohol	16	13	26.8
Hydrogen	21	gas	120.0
Nitroglycerine	40	–	18.2
Sulfur	4	–	9.3
Toluene	16	40	31.3
Vinyl chloride	21	gas	18.6

A. *Toxic materials*: The presence of toxic substances after an incident will make the task of emergency personnel more difficult. The factor applied ranges from 0 for nontoxic materials to 0.8 for substances that can cause death after short exposure.

B. *Subatmospheric pressure*: Allows for the hazard of air leakage into equipment. It is only applied for pressure less than 500 mmHg (0.66 bara).

C. *Operation in or near flammable range*: Covers the possibility of air mixing with material in equipment or storage tanks under conditions where the mixture will be within the explosive range.

D. *Dust explosion*: Covers the possibility of a dust explosion. The degree of risk is largely determined by the particle size. The penalty factor varies from 0.25 for particles above 175 μm to 2.0 for particles below 75 μm.

E. *Relief pressure*: This penalty accounts for the effect of pressure on the rate of leakage should a leak occur. Equipment design and operation become more critical as the operating pressure is increased. The factor to apply depends on the relief device setting and the physical nature of the process material. It is determined from Fig. 2 in the Dow Guide.

F. *Low temperature*: This factor allows for the possibility of brittle fracture occurring in carbon steel or other metals at low temperatures (see Chapter 6 of this book).

G. *Quantity of flammable material*: The potential loss will be greater the greater the quantity of hazardous material in the process or in storage. The factor to apply depends on the physical state and hazardous nature of the process material and the quantity of material. It varies from 0.1 to 3.0 and is determined from Figs. 3, 4, and 5 in the Dow Guide.

H. *Corrosion and erosion*: Despite good design and materials selection, some corrosion problems may arise, both internally and externally. The factor to be applied depends on the anticipated corrosion rate. The severest factor is applied if stress corrosion cracking is likely to occur (see Chapter 6 of this book).

I. *Leakage—joints and packing*: This factor accounts for the possibility of leakage from gaskets, pumps and other shaft seals, and packed glands. The factor varies from 0.1, where there is the possibility of minor leaks, to 1.5 for processes that have sight glasses, bellows, or other expansion joints.

J. *Use of fired heaters*: The presence of boilers or furnaces heated by the combustion of fuels increases the probability of ignition should a leak of flammable material occur from a process unit. The risk involved will depend on the siting of the fired equipment and the flash point of the process material. The factor to apply is determined with reference to Fig. 6 in the Dow Guide.

K. *Hot oil heat exchange system*: Most special heat exchange fluids are flammable and are often used above their flash points, so their use in a unit increases the risk of fire or explosion. The factor to apply depends on the quantity and whether the fluid is above or below its flash point; see Table 5 in the Guide.

L. *Rotating equipment*: This factor accounts for the hazard arising from the use of large pieces of rotating equipment: compressors, centrifuges, and some mixers.

10.6.2 Potential loss

The procedure for estimating the potential loss that would follow an incident is set out in Table 10.8. The first step is to calculate the *damage factor* for the unit. The damage factor depends on the value of the material factor and the process unit hazards factor (F_3 in Fig. 10.3). It is determined using Fig. 8 in the Dow Guide.

An estimate is then made of the area (radius) of exposure. This represents the area containing equipment that could be damaged following a fire or explosion in the unit being considered. It is evaluated from Fig. 7 in the Guide and is a linear function of the F&EI.

An estimate of the replacement value of the equipment within the exposed area is then made and combined with the damage factor to estimate the *base maximum probable property damage* (base MPPD).

The *maximum probable property damage* (MPPD) is then calculated by multiplying the base MPPD by a *loss control credit factor*. The loss control credit factors (Table 10.9) allow for the reduction in the potential loss given by the

TABLE 10.8 Loss control credit factors

Feature	Credit factor range	Credit factor used (2)
1. Process Control Credit Factor (C1)		
a. Emergency Power	0.98	
b. Cooling	0.97–0.99	
c. Explosion Control	0.84–0.98	
d. Emergency Shut-down	0.96–0.99	
e. Computer Control	0.93–0.99	
f. Inert Gas	0.94–0.96	
g. Operating Instructions/Procedures	0.91–0.99	
h. Reactive Chemical Review	0.91–0.98	
i. Other Process Hazard Analysis	0.91–0.98	
C_1 Value(3) : _____		
2. Material Isolation Credit Factor (C2)		
a. Remote Control Valves	0.96–0.98	
b. Dump/Blowdown	0.96–0.98	
c. Drainage	0.91–0.97	
d. Interlock	0.98	
C_2 Value(3) : _____		
3. Fire Protection Credit Factor (C3)		
a. Leak Detection	0.94–0.98	
b. Structural Steel	0.95–0.98	
c. Fire Water Supply	0.94–0.97	
d. Special Systems	0.91	
e. Sprinkler Systems	0.74–0.97	
f. Water Curtains	0.97–0.98	
g. Foam	0.92–0.97	
h. Hand Extinguishers/Monitors	0.93–0.98	
i. Cable Protection	0.94–0.98	
C_3 Value(3) : _____		
Loss Control Credit Factor = C_1 x C_2 x C_3 = _____ Enter on Line 7 in Table 10.9		

(2)For no credit factor enter 1.00.
(3)Product of all factors used.
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TABLE 10.9 Process unit risk analysis summary

1. Fire & Explosion Index (F&El)	
2. Radius of Exposure	(Fig. 7)* ft or m
3. Area of Exposure	ft^2 or m^2
4. Value of Area of Exposure	$MM
5. Damage Factor	(Fig. 8)*
6. Base Maximum Probable Property Damage — (Base MPPD) [4 × 5]	$MM
7. Loss Control Credit Factor	(See earlier)
8. Actual Maximum Probable Property Damage — (Actual MPPD) [6 × 7]	$MM
9. Maximum Probable Days Outage — (MPDO)	(Fig. 9)* days
10. Business Interruption — (Bl)	$MM
(2) For no credit factor enter 1.00.	
(3) Product of all factors used.	

** Refer to Fire & Explosion Index Hazard Classification Guide for details. From Dow (1994).*
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preventive and protective measures incorporated in the design. The Dow Guide should be consulted for details of how to calculate the credit factors.

The MPPD is used to predict the maximum number of days that the plant will be down for repair, the *maximum probable days outage* (MPDO). The MPDO is used to estimate the financial loss due to the lost production: the *business interruption* (BI). The financial loss due to lost business opportunity can often exceed the loss from property damage.

10.6.3 Basic preventive and protective measures

The basic safety and fire protective measures that should be included in all chemical process designs are listed here. This list is based on that given in the Dow Guide, with some minor amendments.

1. Adequate and secure water supplies for firefighting.
2. Correct structural design of vessels, piping, and steel work.
3. Pressure-relief devices.
4. Corrosion-resistant materials and/or adequate corrosion allowances.
5. Segregation of reactive materials.
6. Grounding of electrical equipment.
7. Safe location of auxiliary electrical equipment, transformers, and switch gear.
8. Provision of backup utility supplies and services.
9. Compliance with national codes and standards.
10. Fail-safe instrumentation.
11. Provision for access of emergency vehicles and the evacuation of personnel.
12. Adequate drainage for spills and firefighting water.
13. Insulation of hot surfaces.
14. No glass equipment used for flammable or hazardous materials unless no suitable alternative is available.
15. Adequate separation of hazardous equipment.
16. Protection of pipe racks and cable trays from fire.
17. Provision of block valves on lines to main processing areas.
18. Protection of fired equipment (heaters, furnaces) against accidental explosion and fire.
19. Safe design and location of control rooms.

Note: The design and location of control rooms, particularly with regard to protection against an unconfined vapor explosion, is covered in a publication of the Chemical Industries Association (CIA, 1979).

10.6.4 Mond fire, explosion, and toxicity index

The Mond index was developed from the Dow F&EI by personnel at the ICI Mond division. The third edition of the Dow index, Dow (1973), was extended to cover a wider range of process and storage installations, the processing of chemicals with explosive properties, and the evaluation of a toxicity hazards index. Also included was a

procedure to allow for the offsetting effects of good design and of control and safety instrumentation. Their revised Mond fire, explosion, and toxicity index was discussed in a series of papers by Lewis (1979a, 1979b), which included a technical manual setting out the calculation procedure. An extended version of the manual was issued in 1985, and an amended version published in 1993 (ICI, 1993).

Procedure

The basic procedures for calculating the Mond indices are similar to those used for the Dow index.

The process is first divided into a number of units that are assessed individually.

The dominant material for each unit is then selected and its material factor determined. The material factor in the Mond index is a function of the energy content per unit weight (the heat of combustion).

The material factor is then modified to allow for the effect of general and special process and material hazards, the physical quantity of the material in the process step, the plant layout, and the toxicity of process materials.

Separate fire and explosion indices are calculated. An aerial explosion index can also be estimated to assess the potential hazard of aerial explosions. An equivalent Dow index can also be determined.

The individual fire and explosion indices are combined to give an overall index for the process unit. The overall index is the most important in assessing the potential hazard.

The magnitude of the potential hazard is determined by reference to rating tables, similar to that shown for the Dow index in Table 10.6.

After the initial calculation of the indices (the initial indices), the process is reviewed to see what measures can be taken to reduce the rating (the potential hazard).

The appropriate offsetting factors to allow for the preventive features included in the design are then applied, and final hazard indices are calculated.

Preventive measures

Preventive measures fall into two categories:

1. Those that reduce the number of incidents, such as sound mechanical design of equipment and piping, operating and maintenance procedures, and operator training.
2. Those that reduce the scale of a potential incident, such as measures for fire protection and fixed firefighting equipment.

Many measures will not fit neatly into individual categories but will apply to both.

Implementation

The Mond technique of hazard evaluation is fully explained in the ICI technical manual (ICI 1993), to which reference should be made to implement the method. The calculations are made using a standard form, similar to that used for the Dow index.

10.6.5 Summary

The Dow and Mond indices are useful techniques that can be used in the early stages of a project design to evaluate the hazards and risks of the proposed process.

Calculation of the indices for the various sections of the process will highlight any particularly hazardous sections and indicate where a detailed study is needed to reduce the hazards.

Example 10.1

Evaluate the Dow F&EI for the nitric acid plant illustrated in Chapter 2, Fig. 2.8.

Solution

The calculation is set out on the special form shown in Fig. 10.3(a). Notes on the decisions taken and the factors used are given here.

Unit: Consider the total plant, no separate areas, but exclude the main storages.
Material factor: For ammonia, from the Dow Guide and Table 10.6.

$$\text{MF} = 4.0$$

Note: Hydrogen is present and has a larger material factor (21), but the concentration is too small for it to be considered the dominant material.

General process hazards

A. Oxidizing reaction, factor = 0.5
B. Not applicable
C. Not applicable
D. Not applicable
E. Adequate access would be provided, factor = 0.0
F. Adequate drainage would be provided, factor = 0.0

FIRE & EXPLOSION INDEX

AREA/COUNTRY -	DIVISION -	LOCATION SLIGO	DATE 20 JAN 1997
SITE -	MANUFACTURING UNIT NITRIC ACID	PROCESS UNIT COMPLETE PLANT	
PREPARED BY: RKS	APPROVED BY:(Superintendent) ANOTHER	BUILDING -	
REVIEWED BY:(Management) -	REVIEWED BY:(Technology Center) -	REVIEWED BY:(Safety & Loss Prevention) -	
MATERIALS IN PROCESS UNIT AMMONIA, AIR, OXIDES OF NITROGEN, WATER			
STATE OF OPERATION — DESIGN — START UP ✓ NORMAL OPERATION — SHUTDOWN	BASIC MATERIAL(S) FOR MATERIAL FACTOR AMMONIA		
MATERIAL FACTOR (See Table 1 or Appendices A or B) Note requirements when unit temperature over 140 °F (60 °C)			4

1. General Process Hazards	Penalty Factor Range	Penalty Factor Used(1)
Base Factor	1.00	1.00
A. Exothermic Chemical Reactions	0.30 to 1.25	0.50
B. Endothermic Processes	0.20 to 0.40	
C. Material Handling and Transfer	0.25 to 1.05	
D. Enclosed or Indoor Process Units	0.25 to 0.90	
E. Access	0.20 to 0.35	
F. Drainage and Spill Control _____ gal or cu.m.	0.25 to 0.50	
General Process Hazards Factor (F_1)		1.50
2. Special Process Hazards		
Base Factor	1.00	1.00
A. Toxic Material(s)	0.20 to 0.80	0.60
B. Sub-Atmospheric Pressure (< 500 mm Hg)	0.50	
C. Operation In or Near Flammable Range ___ Inerted ___ Not Inerted		
1. Tank Farms Storage Flammable Liquids	0.50	
2. Process Upset or Purge Failure	0.30	0.80
3. Always in Flammable Range	0.80	
D. Dust Explosion (See Table 3)	0.25 to 2.00	
E. Pressure (See Figure 2) Operating Pressure 103 psig or kPa gauge; Relief Setting 125 psig or kPa gauge		0.35
F. Low Temperature	0.20 to 0.30	
G. Quantity of Flammable/Unstable Material: Quantity _____ lb or kg; H_C = _____ BTU/lb or kcal/kg		
1. Liquids or Gases in Process (See Figure 3)		
2. Liquids or Gases in Storage (See Figure 4)		
3. Combustible Solids in Storage, Dust in Process (See Figure 5)		
H. Corrosion and Erosion	0.10 to 0.75	0.10
I. Leakage – Joints and Packing	0.10 to 1.50	0.10
J. Use of Fired Equipment (See Figure 6)		
K. Hot Oil Heat Exchange System (See Table 5)	0.15 to 1.15	
L. Rotating Equipment	0.50	0.50
Special Process Hazards Factor (F_2)		3.45
Process Unit Hazards Factor (F_1 x F_2) = F_3		5.20
Fire and Explosion Index (F_3 x MF = F&EI)		21

(1) For no penalty use 0.00.

(b)

FIG. 10.3 (A) Fire and Explosion Index calculation form, Example 10.1. *From Dow [1994] reproduced by permission of the American Institute of Chemical Engineers. © 1994 AIChE. All rights reserved.*

Special process hazards

A. Ammonia is highly toxic and likely to cause serious injury, factor = 0.6.
B. Not applicable.
C. Operation always is within the flammable limits, factor = 0.8.
D. Not applicable.
E. Operation pressure 8 atm = 8 × 14.7 − 14.7 = 103 psig. Set relief valve at 20% above the operating pressure (see Chapter 13 of this book) = 125 psig.
From Fig. 2 in the guide, factor = 0.35.
Note: psig = pounds force per square inch, gauge.
F. Not applicable.
G. The largest quantity of ammonia in the process will be the liquid in the vaporizer, say around 500 kg.
Heat of combustion (see Table 10.3) = 18.6 MJ/kg
Potential energy release = 500 × 18.6 = 9300 MJ
$= 9300 \times 10^6/(1.05506 \times 10^3) = 8.81 \times 10^6$ Btu
which is too small to register on Fig. 3 in the Guide, factor = 0.0.
H. Corrosion-resistant materials of construction would be specified, but external corrosion is possible due to nitric oxide fumes, allow minimum factor = 0.1.
I. Welded joints would be used on ammonia service and mechanical seals on pumps. Use minimum factor, as full equipment details are not known at the flowsheet stage, factor = 0.1.
J. Not applicable.
K. Not applicable.
L. Large turbines and compressors used, factor = 0.5.

The index works out at 21: classified as "Light." Ammonia would not normally be considered a dangerously flammable material; the danger of an internal explosion in the reactor is the main process hazard. The toxicity of ammonia and the corrosiveness of nitric acid would also need to be considered in a full hazard evaluation. The process unit risk analysis would be completed when the site for the plant had been determined.

10.7 Hazard and operability studies

A HAZOP study is a systematic procedure for critical examination of the operability of a process. When applied to a process design or an operating plant, it indicates potential hazards that may arise from deviations from the intended design conditions. The technique was developed by the Petrochemicals Division of ICI (see Lawley, 1974) and is now in general use in the chemical and process industries.

The term *operability study* should more properly be used for this type of study, though it is usually referred to as a *hazard and operability study* (HAZOP study). This can cause confusion with the term *hazard analysis* or *process hazard analysis* (PHA), which is a similar but somewhat less rigorous method. Numerous books have been written illustrating the use of HAZOP. Those by Hyatt (2003), CCPS (2000), Kletz (1999), and Crawley and Tyler (2015) give comprehensive descriptions of the technique, with examples.

A brief outline of the technique is given in this section to illustrate its use in process design. It can be used to make a preliminary examination of the design at the flowsheet stage and for a detailed study at a later stage, when a full process description, final flowsheets, P&I diagrams, and equipment details are available. An "as-built" HAZOP is often carried out after construction and immediately before commissioning a new plant.

10.7.1 Basic principles

A formal operability study is the systematic study of the design, vessel by vessel and line by line, using "guide words" to help generate thought about the way deviations from the intended operating conditions can cause hazardous situations.

The seven guide words recommended are given in Table 10.10. In addition to these words, the following words are used in a special way and have the precise meanings given here:

TABLE 10.10 A list of guide words

Guide words	Meanings	Comments
No or Not	The complete negation of these intentions	No part of the intentions is achieved and nothing else happens.
More Less	Quantitative increases or decreases	These refer to quantities and properties such as flow rates or temperatures, as well as activities like "Heat" or "React."
As well as	A qualitative increase	All the design and operating intentions are achieved, together with some additional activity.
Part of	A qualitative decrease	Only some of the intentions are achieved; some are not.
Reverse	The logical opposite of the intention	This is most applicable to activities, for example, reverse flow or chemical reaction. It can also be applied to substances (e.g., "Poison" instead of "Antidote" or "D" instead of "L" optical isomers).
Other than	Complete substitution	No part of the original intention is achieved. Something quite different happens.

Intention: The intention defines how the particular part of the process was intended to operate; the intention of the designer.
Deviations: These are departures from the designer's intention that are detected by the systematic application of the guide words.
Causes: Reasons why, and how, the deviations could occur. Only if a deviation can be shown to have a realistic cause is it treated as meaningful.
Consequences: The results that follow from the occurrence of a meaningful deviation.
Hazards: Consequences that can cause damage (loss) or injury.

The use of the guide words can be illustrated by considering a simple example. Fig. 10.4 shows a chlorine vaporizer, which supplies chlorine at 2 bar to a chlorination reactor. The vaporizer is heated by condensing steam.

Consider the steam supply line and associated control instrumentation. The designer's intention is that steam shall be supplied at a pressure and flow rate to match the required chlorine demand.

Apply the guide word No:

Possible deviation − no steam flow.
Possible causes − blockage, valve failure (mechanical or power), failure of steam supply (fracture of main, boiler shut-down).

Clearly this is a meaningful deviation, with several plausible causes.

Consequences − The main consequence is loss of chlorine flow to the chlorination reactor.

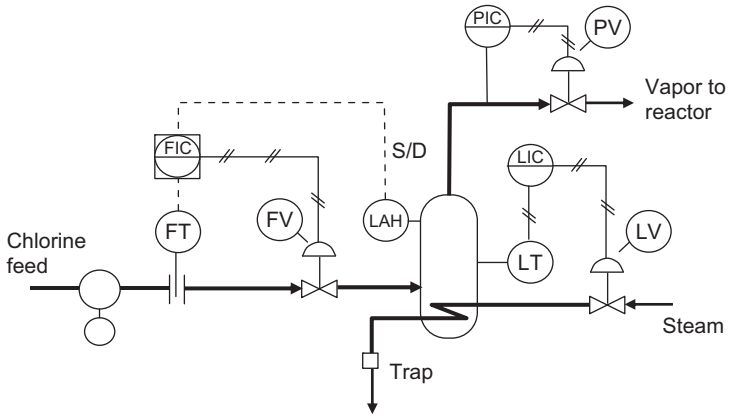


FIG. 10.4 Chlorine vaporizer instrumentation.

The effect of this on the reactor operation would have to be considered. This would be brought out in the operability study on the reactor; it would be a possible cause of no chlorine flow. Because the flow controller does not know that steam flow has been lost, chlorine will continue to be pumped into the vessel until the high-level alarm sounds and the high-level shut-down closes the control valve. A secondary consequence is that the vessel is now filled with liquid chlorine that must be drained to a safe level before operation can be resumed. The operating procedures must include instructions on how to deal with this scenario.

Apply the guide word MORE:

Possible deviation – More steam flow.
Possible cause – Valve stuck open.
Consequences – Low level in vaporizer (this should activate the low-level alarm), higher rate of flow to the reactor.

Note: To some extent the level will be self-regulating, because as the level falls, the heating surface is uncovered.

Hazard – Depends on the possible effect of high flow on the reactor.
Possible deviation – More steam pressure (increase in mains pressure).
Possible causes – Failure of pressure-regulating valves.
Consequences – Increase in vaporization rate. Need to consider the consequences of the heating coil reaching the maximum possible steam system pressure.
Hazard – Rupture of lines (unlikely), effect of sudden increase in chlorine flow on reactor.

A more detailed illustration of the HAZOP method is given in Example 10.2.

10.7.2 Explanation of guide words

It is important to understand the intended meaning of the guide words in Table 10.10. The meaning of the words NO/NOT, MORE, and LESS are easily understood; the NO/NOT, MORE, and LESS could, for example, refer to flow, pressure, temperature, level, and viscosity. All circumstances leading to NO flow should be considered, including reverse flow.

The other words need some further explanation:

AS WELL AS: Something in addition to the design intention, such as impurities, side reactions, ingress of air, or extra phases present.
PART OF: Something missing, only part of the intention realized, such as the change in composition of a stream or a missing component.
REVERSE: The reverse of, or opposite to, the design intention. This could mean reverse flow if the intention were to transfer material. For a reaction, it could mean the reverse reaction. In heat transfer, it could mean the transfer of heat in the opposite direction to what was intended.
OTHER THAN: An important and far-reaching guide word, but consequently more vague in its application. It covers all conceivable situations other than that intended, such as start-up, shut-down, maintenance, catalyst regeneration and charging, and failure of plant services.

When referring to time, the guide words SOONER THAN and LATER THAN can also be used.

10.7.3 Procedure

An operability study would normally be carried out by a team of experienced people, who have complementary skills and knowledge, led by a team leader who is experienced in the technique. The team would include a similar set of experts to an FMEA team, as described in Section 10.5. The team examines the process vessel by vessel, and line by line, using the guide words to detect any hazards.

The information required for the study will depend on the extent of the investigation. A preliminary study can be made from a description of the process and the process flow diagrams. For a detailed, final study of the design, the flowsheets, piping and instrument diagrams, equipment specifications, and layout drawings would be needed. For a batch process, information on the sequence of operation will also be required, such as that given in operating instructions, logic diagrams, and flow charts.

A typical sequence of events is shown in Fig. 10.5. After each line has been studied it is marked on the flowsheet as checked.

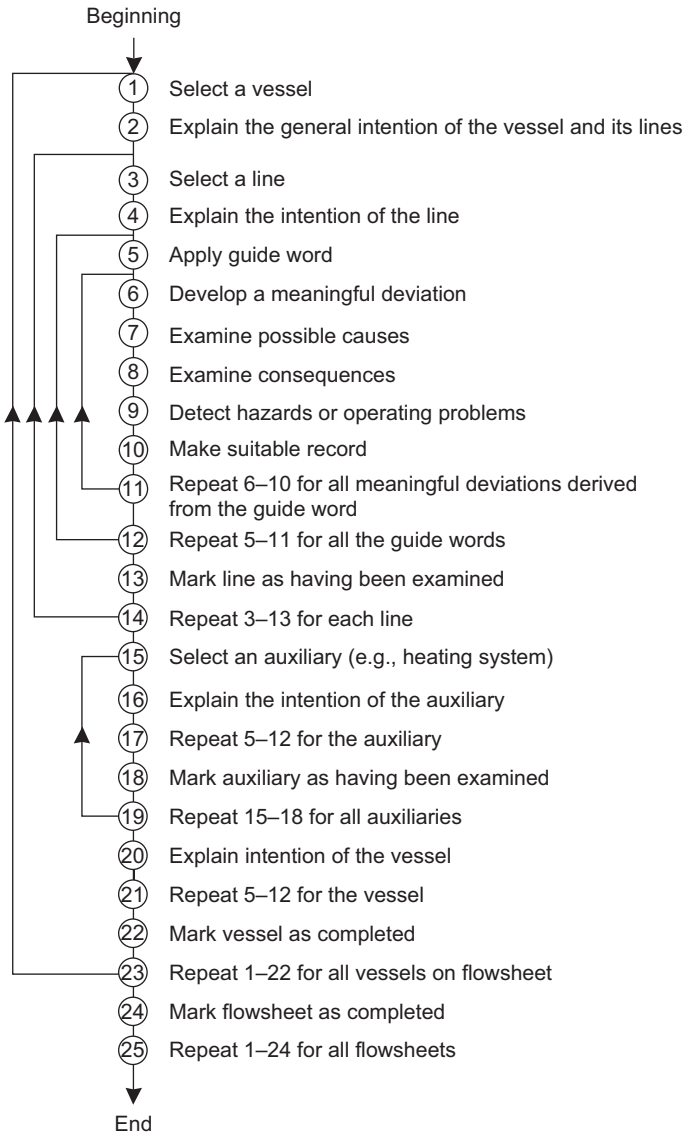


FIG. 10.5 Detailed sequence of an operability study.

A written record is not normally made of each step in the study—only those deviations that lead to a potential hazard are recorded. If possible, the action needed to remove the hazard is decided by the team and recorded. If more information, or time, is needed to decide the best action, the matter is referred to the design group for action or taken up at another meeting of the study team.

When using the operability study technique to vet a process design, the action to be taken to deal with a potential hazard will often be modifications to the control systems and instrumentation: the inclusion of additional alarms, trips, or interlocks. If major hazards are identified, major design changes may be necessary; alternative processes, materials, or equipment should be considered.

Example 10.2

This example illustrates how the techniques used in an operability study can be used to decide the instrumentation required for safe operation. Fig. 10.6(a) shows the basic instrumentation and control systems required for the steady-state operation of the reactor section of the nitric acid process introduced in Fig. 2.8. Fig. 10.6(b) shows the additional instrumentation and safety trips added after making the operability study set out next. The instrument symbols used are explained in Chapter 5.

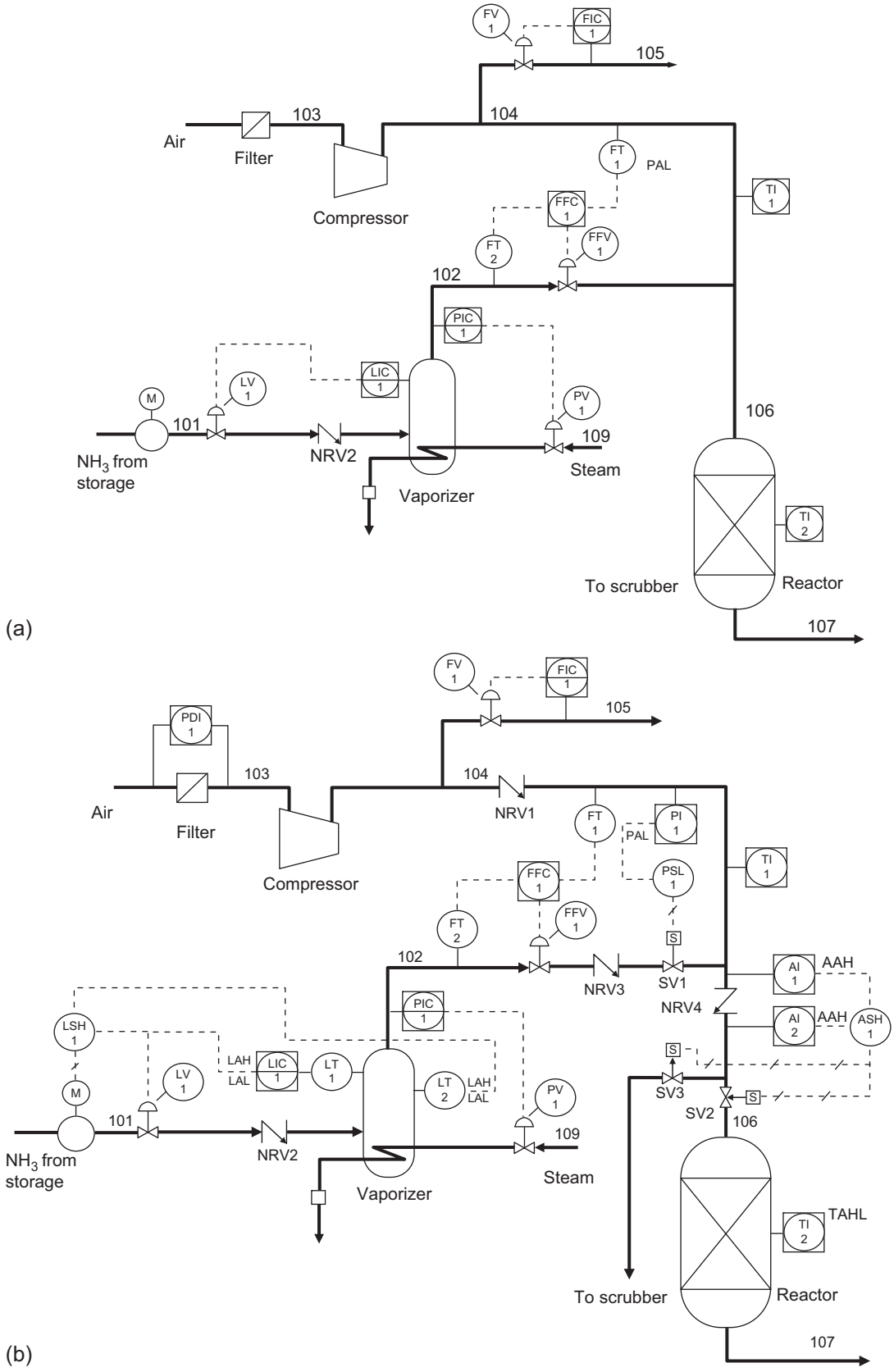


FIG. 10.6 Nitric acid plant reactor section (a) before HAZOP and (b) after HAZOP.

Vessel — **Air Filter**

Intention — to remove particles that would foul the reactor catalyst

Guide Word	Deviation	Cause	Consequences and Action
Line No. 103			
Intention — transfers clear air at atmospheric pressure and ambient temperature to compressor			
LESS OF	Flow	Partially blocked filter	Possible dangerous increase in NH_3 concentration; measure and log pressure differential
AS WELL AS	Composition	Filter damaged, incorrectly installed	Impurities, possible poisoning of catalyst; proper maintenance

Vessel — **Compressor**

Intention — to supply air at 8 bar, 12,000 kg/h, 250 °C, to the mixing tee

Line No. 104			
Intention — transfers air to reactor (mixing tee)			
NO/NONE	Flow	Compressor failure	Possible dangerous NH_3 concentration: pressure indicator with low pressure alarm (PI1) interlocked to shut down NH_3 flow
MORE	Flow	Failure of compressor controls	High rate of reaction, high reactor temperature: high-temperature alarms added to TI2
REVERSE	Flow	Fall in line press. (compressor fails) high pressure at reactor	NH_3 in compressor — explosion hazard: fit nonreturn valve (NRV1); hot wet acid reactor gas-corrosion; fit second valve (NRV4)
Line No. 105			
Intention — transfer secondar air to absorber			
NO	Flow	Compressor failure FV1 failure	Incomplete oxidation, air pollution from absorber vent: operating procedures
LESS	Flow	FV1 plugging failure, FIC1	As no flow

Vessel — **Ammonia vaporizer**

Intention — evaporate liquid ammonia at 8 bar, 25 °C, 731 kg/h

Guide Word	Deviation	Cause	Consequences and Action
Line No. 101			
Intention — transfer liquid NH_3 from storage			
NO	Flow	Pump failure LV1 fails	Level falls in vaporizer: fit low-level alarm on LIC1
LESS	Flow	Partial failure pump/valve	LIC1 alarms
MORE	Flow	LV1 sticking, LIC1 fails	Vaporizer floods, liquid to reactor: fit high-level alarm on LIC1 with automatic pump shut-down. Add independent level transmitter and alarm LT2.
AS WELL AS	Water brine	Leakage into storages from refrigeration	Concentration of NH_4OH in vaporizer: routine analysis, maintenance
REVERSE	Flow	Pump fails, vaporizer press, higher than delivery	Flow of vapor into storages: LIC1 alarms; fit nonreturn valve (NRV2)

—cont'd

Line No. 102			
Intention — transfers vapor to mixing tee			
NO	Flow	Failure of steam flow, FFV1 fails closed,	LIC1 alarms, reaction ceases: considered low flow alarm, rejected — needs resetting at each rate
LESS	Flow	Partial failure or blockage FFV1	As no flow
	Level	LIC1 fails	LT2 backup system alarms
MORE	Flow	FT2/ratio control misoperation	Danger of high ammonia concentration: fit alarm, fit analyzers (duplicate) with high alarm 12% NH_3 (AI1, AI2)
	Level	LIC1 fails	LT2 backup system alarms
REVERSE	Flow	Steam failure	Hot, acid gases from reactor — corrosion: fit nonreturn valve (NRV3)
Line 109 (auxiliary)			
No	Flow	PV1 fails, trap frozen	High level in vaporizer: LIC1 actuated
Vessel — **Reactor**			
Intention — oxidizes NH3 with air, 8 bar, 900 °C			
NO	Flow	NRV4 stuck closed	Fall in reaction rate: fit low temp, alarm on TI2
LESS	Flow	NRV4 partially closed	As NO
	NH3 conc.	Failure to ratio control	Temperatures fall: TI2 alarms (consider low conc. Alarm on AI1, AI2)
MORE	NH3 conc.	Failure of ratio control, air flow restricted	High reactor temp.: TI2 alarms 14% explosive mixture enter reactor — potential for disaster; include automatic shut-down bypass actuated by AI1, AI2, SV2 closes, SV3 opens
	Flow	Control systems failure	High reactor temp.: TI2 alarms
Line No. 107			
Intention — transfer reactor products to waste-heat boiler			
AS WELL AS	Composition	Refractory particles from reactor	Possible plugging of boiler tube: install filter upstream of boiler

The most significant hazard of this process is the probability of an explosion if the concentration of ammonia in the reactor is inadvertently allowed to reach the explosive range, >14%. Note that this is a simplified flow diagram, and a HAZOP based on the full P&I diagram would go into considerably more detail.

Operability study

The sequence of steps shown in Fig. 10.4 is followed. Only deviations leading to action and those having consequences of interest are recorded.

10.8 Quantitative hazard analysis

Methods such as FMEA, HAZOP, and the use of safety indices will identify potential hazards but give only qualitative guidance on the likelihood of an incident occurring and the loss suffered; these are left to the intuition of the team members. In a quantitative hazard analysis, the engineer attempts to determine the probability of an event occurring and the potential cost in terms of injuries, financial loss, etc. The international standard IEC 61508 (1998) defines

the risk of a hazard as the probable rate of occurrence (typically expressed as events per year) multiplied by the degree of severity of the harm caused. If there are no protective systems in place, the inherent risk, R_{np}, is:

$$R_{np} = F_{np} \times C \tag{10.1}$$

where: F_{np} is the inherent frequency of the hazard with no protective system (number of events per year)
C is the impact of the hazard (impact per loss event)

The impact can be stated in terms of injuries, serious injuries, emissions, financial loss, or other measures. The analysis is sometimes repeated with different measures of impact, as the organization may have a different tolerance for risk of injuries than for financial risk.

In most designs, protective systems are added to reduce the risk of a hazard to a tolerable level. The tolerable risk is defined as:

$$R_t = F_t \times C \tag{10.2}$$

where: F_t is the tolerable frequency of the hazard (number of events per year)
R_t is the tolerable risk, also sometimes called the *acceptable risk*

The risk reduction factor of the protective system, ΔR, is defined as the ratio of inherent frequency to tolerable frequency:

$$\Delta R = \frac{F_{np}}{F_t} \tag{10.3}$$

It can be seen that the risk reduction factor is the inverse of the average probability that the protective system will fail when it is called upon to operate (average probability of failure on demand), PFD_{av}:

$$PFD_{av} = \frac{F_t}{F_{np}} = \frac{1}{\Delta R} \tag{10.4}$$

The quantitative hazard analysis can thus be used to set targets for the reliability of the protective system. The reliability of the protective system can then be increased until the desired risk reduction factor is attained. Methods that are used to improve the reliability of the protective system are discussed in Section 10.8.2.

The design of safety instrumented systems for maintaining safe operation of processes is discussed in the international standard IEC 61511, which is adopted as ANSI/ISA-84.00.01-2004 in the United States. For a safety system that must operate on demand (i.e., in response to an initiating event), IEC 61511 states that each safety instrumented function (SIF) must have a safety integrity level (SIL) specified to give the required risk reduction or average probability of failure on demand shown in Table 10.11. A good introduction to the application of the functional safety standards IEC 61508 and 61511 and the development of safety instrumented systems is given by King (2007). The book by Cameron and Raman (2005) is an extensive guide to risk management systems.

10.8.1 Fault trees

Incidents usually occur through the coincident failure of two or more items: failure of equipment, control systems and instruments, and misoperation. The sequence of events leading to a hazardous incident can be shown as a fault tree (logic tree), such as that shown in Fig. 10.7. This figure shows the set of events that could lead to a pressure vessel rupture. The AND symbol is used where all the inputs are necessary before the system fails, and the OR symbol where failure of any input, by itself, would cause failure of the system. A fault tree is analogous to the type of logic

TABLE 10.11 Safety integrity levels in demand mode of operation (IEC 61511)

Safety integrity level (SIL)	Target average probability of failure on demand (PFD_{av})	Target risk reduction factor (ΔR)
4	$\geq 10^{-5}$ to $<10^{-4}$	>10,000 to ≤100,000
3	$\geq 10^{-4}$ to $<10^{-3}$	>1000 to ≤10,000
2	$\geq 10^{-3}$ to $<10^{-2}$	>100 to ≤1000
1	$\geq 10^{-2}$ to $<10^{-1}$	>10 to ≤100

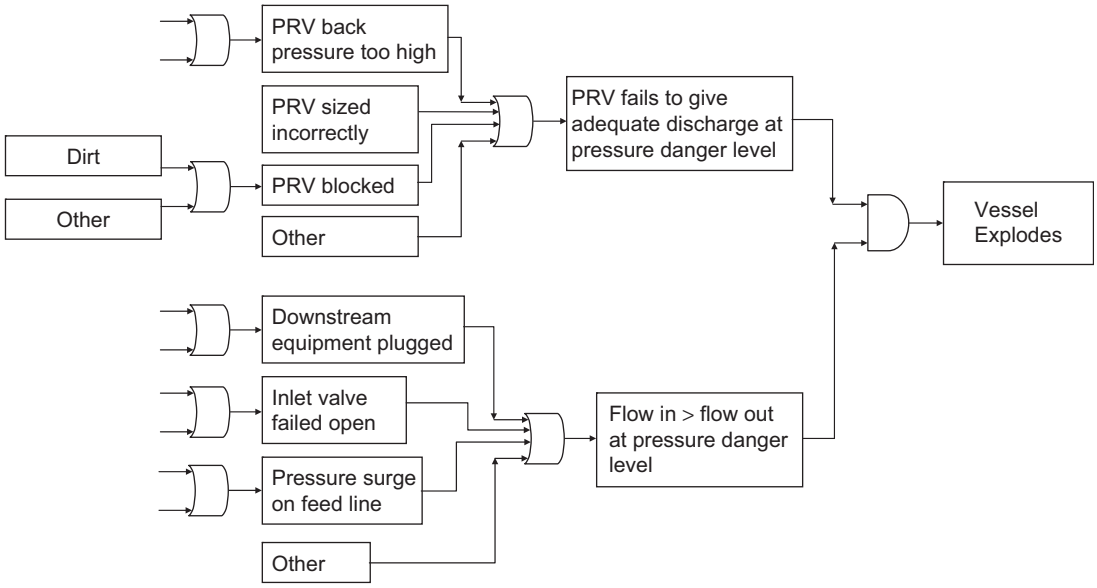


FIG. 10.7 Fault tree for failure of a pressure vessel.

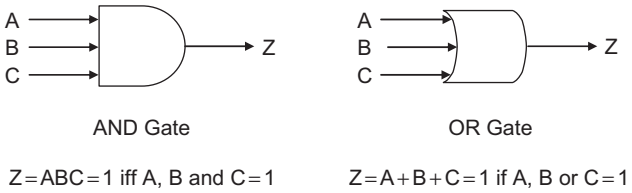


FIG. 10.8 Logic symbols for AND and OR.

diagram used to represent computer operations, and the symbols are analogous to logic AND and OR gates (Fig. 10.8). It can be seen from Fig. 10.7 that failure of the vessel will only occur if there is a cause of overpressure AND a failure of the pressure relief valve (PRV) to respond adequately. These in turn have several possible causes, which may also have possible causes. Each chain of causality should be pursued to the root cause, and the diagram in Fig. 10.7 is incomplete.

The fault trees for even a simple process unit will be complex, with many branches. Fault trees are used to make a quantitative assessment of the likelihood of failure of a system using data on the reliability of the individual components of the system.

Once the fault tree for a subsection of the process has been developed, it can be used to improve the reliability of the design by introducing additional redundant instrumentation. Because a hazardous condition usually requires the failure of one or more devices, introducing additional parallel devices reduces the likelihood of a failure as long the devices do not have a common mode of failure. The quantitative analysis of the likelihood of an event can be used to determine the level of system redundancy that is required to reduce the likelihood to an acceptably low value.

Event trees are a similar way of representing the same information, but there is not sufficient space to present both methods here; see Mannan (2012) or CCPS (2008).

10.8.2 Equipment reliability

When a fault tree has been constructed, it can be used to estimate the probability of the system failing if the probabilities of the events in the fault tree can be estimated. In most cases, this requires a good understanding of the reliability of instruments, alarms, and safety devices, because these devices would be expected to maintain the process in a safe condition.

If the failure rate, λ, is the number of occasions per year that a protective system develops a fault (yr^{-1}) and the time interval between tests of the device is τ years, then intuitively, the device on average fails halfway between tests. The probability that the device is inactive and will fail on demand (also known as the *fractional dead time*) is then approximately:

$$\phi = \frac{\lambda \tau}{2} \tag{10.5}$$

If the demand rate, δ, is the number of occasions per year that the protective device is actuated then the hazard rate, *F*, is:

$$F = \delta \phi = \frac{\delta \lambda \tau}{2} \tag{10.6}$$

The intuitive result in Equation 10.6 is true if and only if δλ, λτ, and δτ are all $<< 1$. For a more rigorous analysis of reliability see Chapters 7 and 13 of Mannan (2012). It can be seen that for a simple system with a single device, the demand rate is the inherent frequency of the hazard, $\delta = F_{np}$, and the probability of the device being inactive is the average probability of failure on demand, $\Phi = PFD_{av}$. Equations 10.6 and 10.4 are therefore equivalent.

The hazard rate can be reduced by using more reliable equipment (lower value of λ), conducting more frequent testing (lower τ), or making improvements that lead to steadier operation (lower δ). Alternatively, two protective systems in parallel can be installed, in which case the hazard rate becomes:

$$F = \frac{4}{3} \delta \phi_A \phi_B \tag{10.7}$$

where: Φ_A is the fractional dead time for system A
Φ_B is the fractional dead time for system B and is subject to the same conditions listed earlier

Example 10.3

Laboratory test data for a trip system shows a failure rate of 0.2 per year. If the demand rate is once every 2 years and the test interval is 6 months, what is the hazard rate? Should a parallel system be installed?

$$\text{Fractional dead time, } \phi = \frac{\lambda\delta}{2} = \frac{0.2 \times 0.5}{2} = 0.05 \tag{10.5}$$

Hazard rate for single system, $F = \delta \Phi = 0.5 \times 0.05 = 0.025$ (i.e., once in every 40 years).

Many plants operate for more than 20 years, so this is probably too high a failure rate to be acceptable. If two systems are used in parallel then:

$$F = \frac{4}{3}\delta\phi_A\phi_B = \frac{4}{3} \times 0.5 \times 0.05 \times 0.05 = \underline{1.67 \times 10^{-3}} \text{ or once in 600 years.}$$

Two systems in parallel should be used, or alternatively, the test frequency could be increased to, say, once every 2 months, giving a more acceptable failure rate of once in every 120 years. Whether the test frequency could be increased will depend on the extent to which testing the device disrupts plant operations. On a large plant with many safety trips and interlocks, it may not be possible to test every system on a frequent basis.

The data on probabilities given in this example are for illustration only and do not represent actual data for these components. Some quantitative data on the reliability of instruments and control systems are given by Mannan (2012). Examples of the application of quantitative hazard analysis techniques in chemical plant design are given by Wells (1996) and Prugh (1980).

The CCPS of the American Institute of Chemical Engineers has published a comprehensive and authoritative guide to quantitative risk analysis (CCPS, 1999). The CCPS has also collected extensive data on device reliability (see CCPS, 1989).

Several other texts are available on the application of risk analysis techniques in the chemical process industries; see CCPS (2000), Frank and Whittle (2001), Cameron and Raman (2005), Crowl and Louvar (2019), Arendt and Lorenzo (2000), Kales (1997), Dodson and Nolan (1999), Green (1983), Kletz (1999), and Crawley and Tyler (2015).

10.8.3 Tolerable risk and safety priorities

If the consequences of an incident can be predicted quantitatively (property loss and the possible number of fatalities), then a quantitative assessment can be made of the risk using Equation 10.1.

If the loss can be measured in money, the cash value of the risk can be compared with the cost of safety equipment or design changes to reduce the risk. In this way, decisions on safety can be made in the same way as other design decisions: to give the best return on the money invested.

Hazards invariably endanger life as well as property, and any attempt to make cost comparisons will be difficult and controversial. It can be argued that no risk to life should be tolerated; however, resources are always limited, and some way of establishing safety priorities is needed.

One approach is to compare the risks, calculated from a hazard analysis, with risks that are generally considered acceptable, such as the average risks in the particular industry and the kind of risks that people accept voluntarily. One measure of the risk to life is the "Fatal Accident Frequency Rate" (FAFR), defined as the number of deaths per 10^8 working hours. This is equivalent to the number of deaths in a group of 1000 people over their working lives. The FAFR can be calculated from statistical data for various industries and activities; some of the published values are shown in Tables 10.12 and 10.13. Table 10.12 shows the relative position of the chemical industry compared with other industries; Table 10.13 gives values for some of the risks that people accept voluntarily.

In the chemical process industries, it is generally accepted that risks with an FAFR greater than 0.4 (one-tenth of the average for industry) should be eliminated as a matter of priority, with the elimination of lesser risks depending on the resources available; see Kletz (1977a). This criterion is for risks to employees; for risks to the general public (undertaken involuntarily), a lower criterion must be used. In the UK, the Health and Safety Executive (HSE) has developed the "as low as reasonably practicable" (ALARP) principle, under which owners can operate a plant in a region defined as tolerable risk as long as they can demonstrate that they have achieved the lowest risk possible, taking into account cost versus risk reduction. The tolerable risk region is defined as a fatality frequency of 10^{-3} to 10^{-6} per person, per year for workers and 10^{-4} to 10^{-6} per person, per year for the general public; see Schmidt (2007). The level of risk to which the public outside the factory gate should be exposed by plant operations will always be a matter of debate and controversy. Kletz (1977b) suggested that a hazard can be considered acceptable if the average risk is less than 1 in 10 million per person, per year. This is an order of magnitude lower than the UK HSE guideline and is equivalent to a FAFR of 0.001—about the same as the chance of being struck by lightning. Additional guidelines on

TABLE 10.12 FAFR for some industries for the period 1978–1990

Industry	FAFR
Chemical industry	1.2
UK manufacturing	1.2
Deep sea fishing	4.2

TABLE 10.13 FAFR for some nonindustrial activities

Activity	FAFR
Staying at home	3
Traveling by rail	5
Traveling by bus	3
Traveling by car	57
Traveling by air	240
Traveling by motorcycle	660
Rock climbing	4000

Source: Brown (2004).

setting tolerable risk are given by Schmidt (2007). There is currently no accepted national guideline on tolerable risk in the United States or Canada.

For further reading on the subject of tolerable risk and risk management, see Cox and Tait (1998) and Lowrance (1976).

10.8.3 Computer software for quantitative risk analysis

The assessment of the risks and consequences involved in the planning and operation of a major plant site is a daunting task.

In industrial practice, the safety instrumented systems that are used are more complex than the simple systems described earlier. If two instruments are used in parallel, with either instrument able to activate a shut-down (a "one out of two" system, denoted 1oo2), then the probability of failure on demand is reduced, as illustrated in Example 10.3, but the likelihood of a spurious shut-down due to instrument failure is doubled. The instrument engineer can overcome this problem by using three instruments with a voting policy that requires two out of three of the instruments to activate before a shut-down is caused (2oo3 voting). The use of programmable logic controllers, distributed control systems, and device communication methods such as Fieldbus means that the reliability of many electrical, electronic, and software components must also be considered in the analysis. Credit can also be taken for the performance of the BPCS as a layer of safety protection (IEC 61511). The calculations soon become too complex to be carried out without using a computer.

The methodology of the classical method of quantitative risk analysis is shown in Fig. 10.9. First, the likely frequency of failure of equipment, pipelines, and storage vessels must be predicted using the techniques described earlier. The probable magnitude of any discharges must then be estimated and the consequences of failure evaluated: fire, explosion, or toxic fume release. Other factors, such as site geography, weather conditions, site layout, and safety management practices, must be taken into consideration. The dispersion of gas clouds can be predicted using suitable models. This methodology enables the severity of the risks to be assessed. Limits have to be agreed on the acceptable risks, such as the permitted concentrations of toxic gases. Decisions can then be made on the location of plant equipment (see Chapter 11), on the suitability of a site location, and on emergency planning procedures.

The comprehensive and detailed assessment of the risks required for a "safety case" can only be satisfactorily carried out for major installations with the aid of computer software. Programs for quantitative risk analysis have been developed by consulting firms that specialize in safety and environmental protection. Typical of the software available is the SAFETI (Suite for Assessment of Flammability Explosion and Toxic Impact) suite of programs developed by DNV GL (www.dnvgl.com). These programs were initially developed for the authorities in the Netherlands as a response

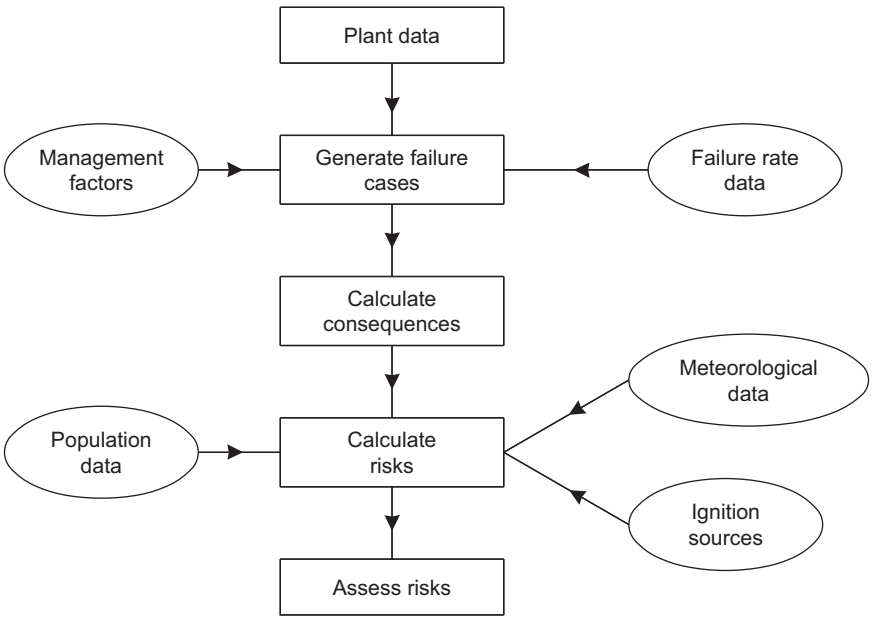


FIG. 10.9 Quantitative risk assessment procedure.

to the Seveso Directives of the EU. The programs have subsequently been developed further and extended and are widely used in the preparation of safety cases; see Pitblado et al. (1990). Other examples include PHAWorks and FaultrEASE from Chempute Software (www.chempute.com), FTA-Pro and PHA-Pro from Sphera (www.sphera.com/pha-pro-software), RENO and BlockSim7 from Reliasoft (www.reliasoft.com), and LOGAN from Reliass (www.reliability-safety-software.com). These and other programs for fault tree analysis, HAZOP, process hazard analysis, and quantitative risk analysis are easily found by searching online, and most chemical companies license one of these programs. Some of the programs offer free trial versions and reduced-cost student subscriptions.

Computer programs can be used to investigate a range of possible scenarios for a site; but as with all computer software used in design, they should not be used without caution and judgment. They would normally be used with the assistance and guidance of the consulting firm supplying the software. With intelligent use, guided by experience, such programs can indicate the magnitude of the likely risks at a site and allow sound decisions to be made when licensing a process operation or granting planning permission for a new installation.

10.9 Pressure relief

Pressure-relief devices are an essential requirement for the safe use of pressure vessels. Pressure-relief devices provide a mechanical means of ensuring that the pressure inside a vessel cannot rise to an unsafe level. All pressure vessels within the scope of Section VIII of the ASME Boiler and Pressure Vessel Code must be fitted with a pressure-relief device. The purpose of the pressure-relief device is to prevent catastrophic failure of the vessel by providing a safe means of relieving overpressure if the pressure inside the vessel exceeds the maximum allowable working pressure.

Three different types of relief devices are commonly used:

- *Directly actuated valves*: Weight or spring-loaded valves that open at a predetermined pressure and that normally close after the pressure has been relieved. The system pressure provides the motive power to operate the valve.
- *Indirectly actuated valves*: Pneumatically or electrically operated valves that are activated by pressure-sensing instruments.
- *Bursting discs*: Thin discs of material that are designed and manufactured to fail at a predetermined pressure.

Relief valves are normally used to regulate minor excursions of pressure; bursting discs are used as safety devices to relieve major overpressure. Bursting discs are often used in conjunction with relief valves to protect the valve from corrosive process fluids during normal operation. The design and selection of relief valves is discussed by Morley (1989a,b) and is also covered by the pressure vessel standards (see later). Bursting discs are discussed by Mathews (1984), Asquith and Lavery (1990), and Murphy (1993). The discs are manufactured in a wide range of common engineering steels and alloys as well as a variety of materials for use in corrosive conditions, such as impervious carbon, gold, and silver, and suitable discs can be found for use with all process fluids. Bursting discs and relief valves are proprietary items, and the vendors should be consulted when selecting suitable types and sizes.

Selection and sizing of the relief device are the responsibility of the end user of the pressure vessel. Rules for the selection and sizing of pressure-relief devices are given in the ASME BPV Code Sec. VIII D.1 Parts UG-125 to UG-137 and D.2 Part AR.

Under the rules given in ASME BPV Code Sec. VIII D.1, the primary pressure-relief device must have a set pressure not greater than the maximum allowable working pressure of the vessel. The primary relief device must be sized to prevent the pressure from rising 10% or 3 psi (20 kPa), whichever is greater, above the maximum allowable working pressure (MAWP). If secondary relief devices are used, their set pressure must not be greater than 5% above the maximum allowable working pressure. When multiple relief devices are used, their combined discharge must be adequate to prevent the vessel pressure from rising more than 16% or 4 psi (30 kPa), whichever is greater, above the maximum allowable working pressure. In a relief scenario where the pressure vessel is exposed to an external fire, the relief device or devices must prevent the vessel pressure from increasing to more than 21% above the maximum allowable working pressure.

Pressure-relief devices must be constructed, located, and installed such that they can be easily inspected and maintained. They are normally located at the top of a vessel in a clean, free-draining location. They must be located on or close to the vessel that they are protecting.

10.9.1 Pressure-relief scenarios

Overpressure will occur whenever mass, moles, or energy accumulate in a contained volume or space with a restricted outflow. The rate at which material or energy accumulates determines the pressure rise. If the process control system is not able to respond quickly enough, the pressure-relief device must be activated before the vessel ruptures, explodes, or suffers some other catastrophic loss of containment.

The first step in designing a pressure-relief system is to evaluate the possible causes of overpressure to determine the rate of pressure accumulation associated with each and hence estimate the relief load (the flow rate that must be discharged through the relief device). The API Standard 521 suggests the following causes:

Blocked outlet	Chemical reaction	Electric power loss
Utility failure	External fire	Accumulation of noncondensable species
Cooling or reflux failure	Abnormal heat input	Failure of automatic controls
Inadvertent valve opening	Operator error	Loss of heat in series fractionation
Loss of fans	Check valve failure	Volatile material entering system
Steam or water hammer	Internal explosion	Heat exchanger tube failure
Adsorbent flow failure	Overheating a liquid full system	

This list is not exhaustive, and the design engineers should always brainstorm for additional scenarios and review the results of FMEA, HAZOP, HAZAN, or other process safety analyses.

In evaluating relief scenarios, the design engineer should consider sequential events that result from the same root-cause event, particularly when these can increase the relief load. For example, the loss of electric power in a plant that carries out a liquid-phase exothermic reaction could have the following impacts:

1. Failure of all or part of the automatic control system.
2. Loss of cooling due to failure of cooling water pumps or air coolers.
3. Loss of mixing in the reactor due to failure of the stirrer, leading to localized runaway reaction.

Because these have a common cause, they should be considered as simultaneous events for that cause. If two events do not share a common cause, then the probability that they will occur simultaneously is remote and is not usually considered (API STD 521, 3.2). Root-cause events such as power loss, utility loss, and external fire will often cause multiple other events and hence large relief loads.

The rate at which pressure accumulates is also affected by the response of the process control system. API STD 521 recommends that instrumentation be assumed to respond as designed if it increases the relieving requirement, but no credit should be taken for instrumentation response if it reduces the relieving requirement. For example in Fig. 10.10(a), if the outlet control valve becomes blocked and the pressure in the vessel rises, the flow from the pump will initially decrease because of the higher back-pressure. The flow controller will compensate for this by

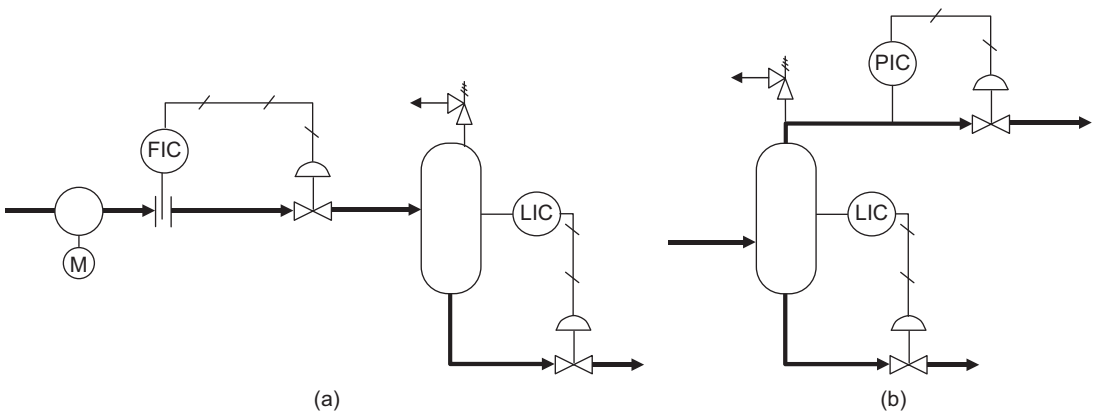


FIG. 10.10 Instrumentation response to pressure-relief scenarios: (a) Instrumentation response increases relieving load. (b) Instrumentation response would reduce relieving load, but API RP 521 recommends taking no credit for instrumentation response.

opening the flow control valve to try to maintain a constant flow rate and will consequently increase the relieving load. The design engineer should assume that the instrumentation responds as designed and the flow rate remains constant. In Fig. 10.10(b), if the outlet control valve becomes blocked, the pressure controller will continue opening the pressure control valve until it is fully open. This provides an alternative outflow and reduces the relieving load, but according to API STD 521 this response should not be considered.

Heat exchangers and other vessels with internal compartments must also be protected from overpressure in the case of an internal failure. This is of particular importance for shell and tube type exchangers, as the common design practice is to put the higher-pressure fluid on the tube side. This saves costs in constructing the shell and obviates sizing the tubes to withstand a high compressive load due to external pressure. If the tube side is at higher pressure, then in the event of a tube or tubesheet failure, the shell will be exposed to the higher tube-side pressure.

Both API STD 521 and ASME BPV Code Section VIII allow multiple vessels connected together to be considered as a single unit for relief scenarios, provided that there are no valves or restriction orifices between the vessels and that the design considers the full relieving load of the system (ASME BPV Code Sec. VIII D.1 UG-133).

10.9.2 Pressure-relief loads

The rate at which pressure accumulates can be estimated by making non−steady-state mass, mole, and energy balances around the vessel or system:

$$\text{in} + \text{formed by reaction} = \text{out} + \text{accumulation} \tag{10.8}$$

Because liquids have very low compressibility, pressure vessels are seldom operated entirely filled with liquid, because small accumulations of material would cause large surges in pressure. Instead, it is common practice to operate with a "bubble" of vapor (often nitrogen) at the top of the vessel. The mass balance equation can then be rearranged into an equation for the rate of change of pressure of this gas with time.

For example, consider a vessel of total volume V m^3 that is normally operated 80% full of liquid on level control, as in Fig. 10.10(a), and is fed with a flow rate v m^3/s of liquid. If the volume of liquid in the vessel is V_L, then if the outlet becomes blocked and the liquid is assumed to be incompressible, then the change in the volume of the liquid is:

$$\frac{dV_L}{dt} = v \tag{10.9}$$

where t = time, s

The volume occupied by vapor, $V_G = V - V_L$, so:

$$\frac{dV_G}{dt} = -\frac{dV_L}{dt} = -v \tag{10.10}$$

If there is no vapor flow in or out of the vessel, then assuming the vapor behaves as an ideal gas:

$$\mathrm{V_G} = \mathrm{nRT/P} \tag{10.11}$$

where n = number of moles in of gas in the vessel, mol
R = ideal gas constant, J/mol.K
T = temperature, K
P = pressure, N/m^2

If the temperature is constant (which is valid for a blocked outlet relief scenario), then until the relief valve opens:

$$\frac{dP}{dt} = nRT\frac{d}{dt}\left(\frac{1}{V_G}\right) = -\frac{nRT}{V_G^2}\frac{dV_G}{dt} = \frac{P^2 v}{nRT} \tag{10.12}$$

Equation 10.12 can be used to estimate the rate of pressure accumulation.

When the relief valve opens, it allows vapor to discharge at a flow rate, w kg/s. The number of moles of vapor in the vessel is then given by:

$$\frac{dn}{dt} = -\frac{1000\,w}{M_w} \tag{10.13}$$

where M_w is the average molecular weight of the vapor, g/mol

The equation for the rate of change of pressure becomes:

$$\frac{dP}{dt} = RT\frac{d}{dt}\left(\frac{n}{V_G}\right) = \frac{RT}{V_G^2}\left(V_G\frac{dn}{dt} - n\frac{dV_G}{dt}\right)$$
$$= \frac{P^2}{nRT}\left(v - \frac{1000\,RTw}{M_w\,P}\right) \tag{10.14}$$

If the relief valve is sized correctly, then the maximum pressure that can accumulate is 110% of the maximum allowable working pressure, P_m (ASME BPV Code Sec. VIII D.1 UG-125). At this point there is no further accumulation of pressure and $dp/dt = 0$; hence:

$$\frac{1000\,RTw}{M_w \times 1.1P_m} = v \tag{10.15}$$

and the required relief load is:

$$w = \frac{1.1P_m\,M_w v}{1000\,RT} \tag{10.16}$$

Equation 10.16 applies as long as only vapor is vented from the vessel. Once the vapor has been displaced by liquid, then the relief load must be the liquid flow rate. If a two-phase mixture is vented, then the calculation becomes more complex.

In most cases the governing relief scenario includes both material and heat input into the system and typically also includes vaporization of material, reaction, and two-phase flow. Such systems are much more difficult to describe using simple differential algebraic models, and the current industrial practice is to use dynamic simulation models for these cases. Dynamic models can be built in any of the commercial process simulators that have this capability. The AIChE Design Institute for Emergency Relief Systems (DIERS) also licenses software called SuperChems (formerly SAFIRE) that is written specifically for pressure-relief system design and incorporates the DIERS-recommended methods and research findings for multiphase, reacting, and highly nonideal systems.

For some relief scenarios, correlations have been established for the relieving load. For the external fire case, API STD 521 (Section 3.15.2) gives:

$$Q = 21000\;F_e\,A_w^{0.82} = w_f\,\Delta H_{vap} \tag{10.17}$$

where Q = heat input due to fire, BTU/hr
F_e = environmental factor
A_w = internal wetted surface area, ft^2
w_f = fire case relieving load, lb/hr
ΔH_{vap} = heat of vaporization, BTU/lb

The environmental factor F_e allows for insulation on the vessel. It is equal to 1.0 for a bare vessel or if the insulation can be stripped off by a liquid jet. The correlation in Equation 10.17 assumes good general design practice and site layout, including use of sewers and trenches or the natural slope of the land to control run-off so that pools do not form. Other formulae for the rate of heat input and relief load are given by ROSPA (1971) and NFPA 30. Local safety regulations and fire codes should be consulted to determine the appropriate method to use in any particular design.

Design codes and standards such as API STD 521 and the DIERS Project Manual (Fisher et al., 1993) should be consulted for other correlations and recommended methods for calculating relief loads. The DIERS Project Manual also discusses calculation of relief loads for underpressure scenarios (see Section 10.9.5).

10.9.3 Design of pressure-relief valves

Spring-loaded relief valves

The most commonly used relief device is the conventional spring-loaded relief valve shown in Fig. 10.11. This design of valve is available in the widest range of sizes and materials (API STD 526, BS EN ISO 4126-1).

In a conventional relief valve the pressure force acts on a disk that is held against a seating surface by a spring. The compression of the spring can be adjusted using an adjusting screw so that the spring force is equal to the pressure force at the valve set pressure.

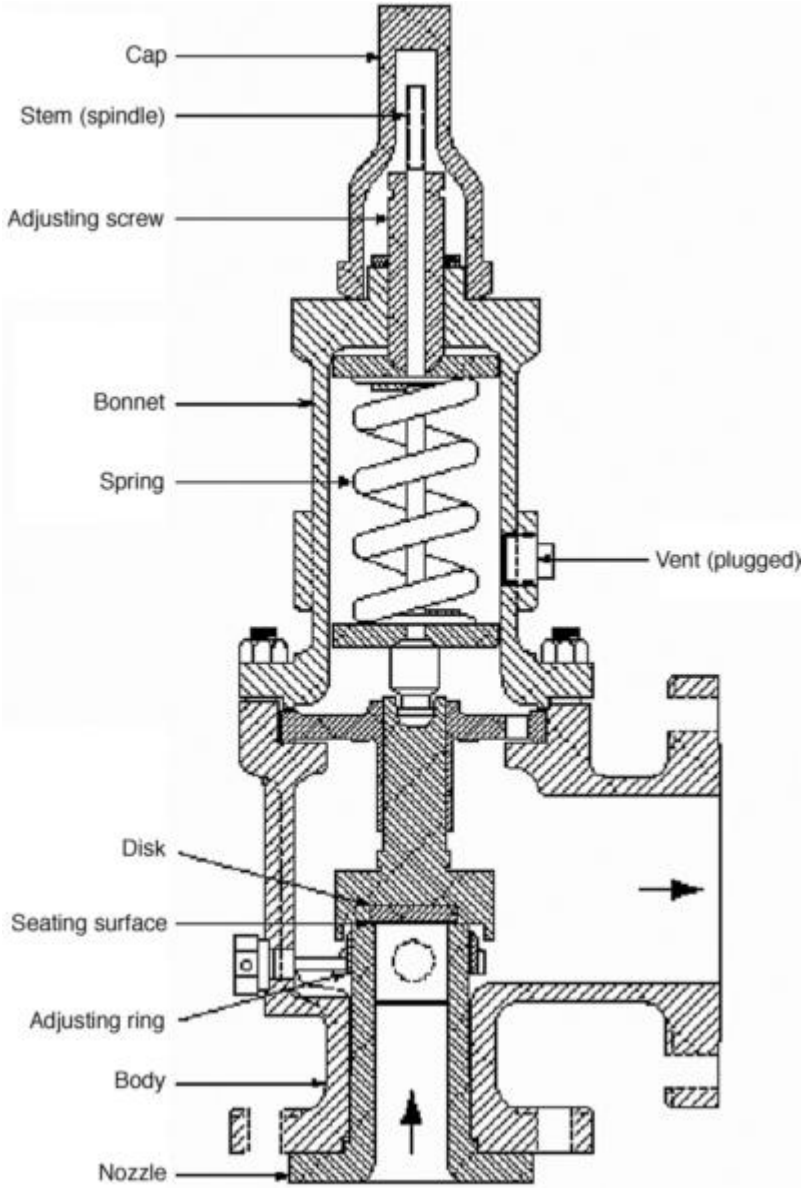


FIG. 10.11 Conventional spring-loaded relief valve. *Reproduced with permission from API Recommended Practice 520.*

The pressure flow response of a conventional relief valve is illustrated schematically in Fig. 10.12. When the pressure in the vessel reaches 92% to 95% of the set pressure, a spring-loaded relief valve in a gas or vapor service begins to "simmer" and leak gas. Leakage can be reduced by lapping the disk and seating surface to a high degree of polish, using elastomeric seals (at low temperatures only), or using a high-pressure differential between the operating pressure and set pressure. When the set pressure is reached, the valve "pops" and the disk lifts from the seat. The disk and seat are shaped such that the force on the disk continues to increase until the valve is fully open, at which point the flow rate is limited only by the bore area of the seating surface and not by the gap between the seating surface and the disk. At this point the design flow rate is achieved and there should be no further pressure accumulation.

When the pressure falls sufficiently, the spring force can overcome the forces due to the flowing fluid, and the valve reseats. Reseating usually occurs at a lower pressure than the set pressure, giving a different curve for blowdown.

The capacity and lift pressure of a conventional spring-loaded relief valve are affected by the back-pressure in the downstream relief system. The back-pressure exerts forces that are additive to the spring force. Where back-pressure is known to fluctuate or accumulate, balanced pressure relief valves that incorporate a bellows or other means of

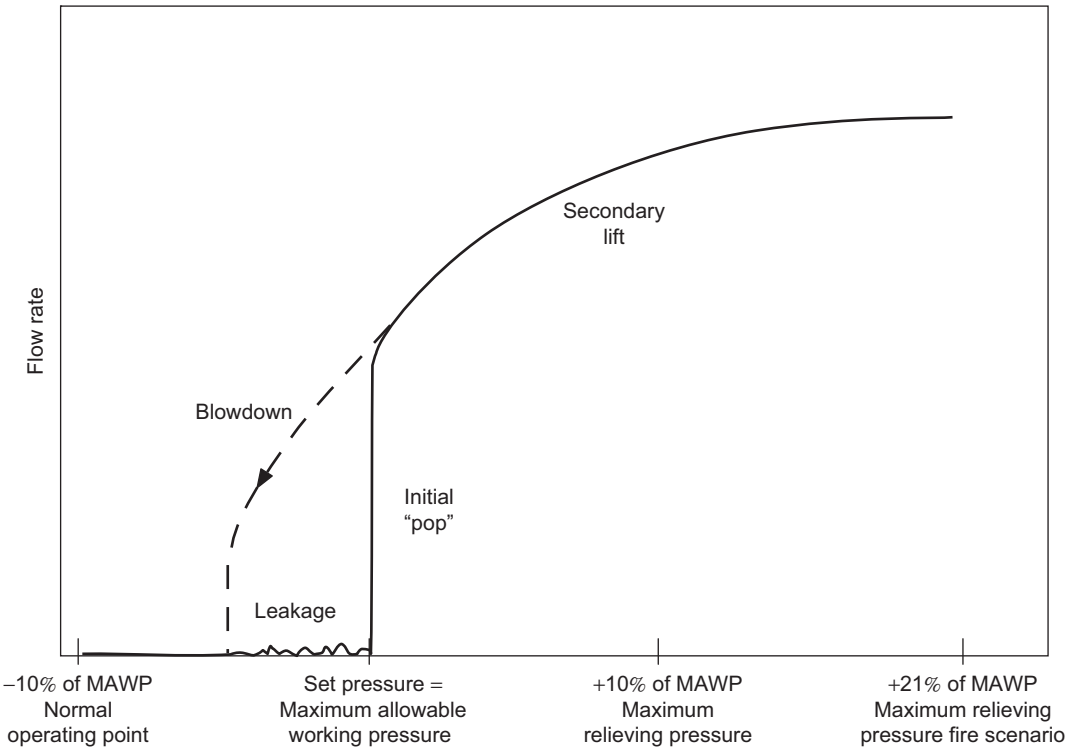


FIG. 10.12 Pressure–flow response of a conventional spring-loaded relief valve.

compensating for back-pressure should be used (see API STD 520 for details). This is particularly important when multiple devices are relieved into the same vent or flare system, as common-cause relief scenarios such as power loss can trigger multiple relief events and send a lot of material into the vent or flare system, increasing the back-pressure acting on the relief valves.

Pilot-operated relief valves

Pilot-operated relief valves are designed to overcome some of the major drawbacks of conventional spring-loaded relief valves. In a pilot-operated relief valve, the spring and disk are replaced by a piston, as shown in Fig. 10.13. A narrow-bore pipe known as a *pilot supply line* connects from the top of the piston to the relief valve inlet via a secondary (pilot) valve of the spring-loaded type. In normal operation both sides of the valve see the same pressure, but because the top surface area of the piston is greater than the area of the seat, the downward force is greater and the valve remains closed. When the pressure exceeds the set pressure, the pilot valve opens and pressure above the piston is lost. This causes the piston to lift, and the valve opens. The pilot valve vent can be exhausted to atmosphere or to the main valve outlet, depending on the containment requirements for the process fluid.

The pressure-flow response of a pilot-operated relief valve is illustrated schematically in Fig. 10.14. Leakage is eliminated, and there is no blowdown.

Pilot-operated relief valves are used in applications that require a low differential between operating pressure and set pressure (for example, revamps where the vessel is now operated closer to the maximum allowable working pressure or vessels operating below 230 kPa or 20 psig): high-pressure services (above 69 bara or 1000 psig) and cases where low leakage is required. They are not available in as broad a range of metallurgies as spring-loaded relief valves. Pilot-operated relief valves are also restricted to lower-temperature applications, as they typically use elastomeric materials to make a seal between the piston and its housing. More details of pilot-operated relief valves are given in BS EN ISO 4126-4.

Sizing relief valves

Guidelines for sizing relief valves are given in API STD 520 and BS EN ISO 4126. Different design equations are recommended for vapor, liquid, steam, or two-phase flows. Sizing methods are also discussed in the DIERS Project Manual (Fisher et al., 1993) and the book by CCPS (2017).

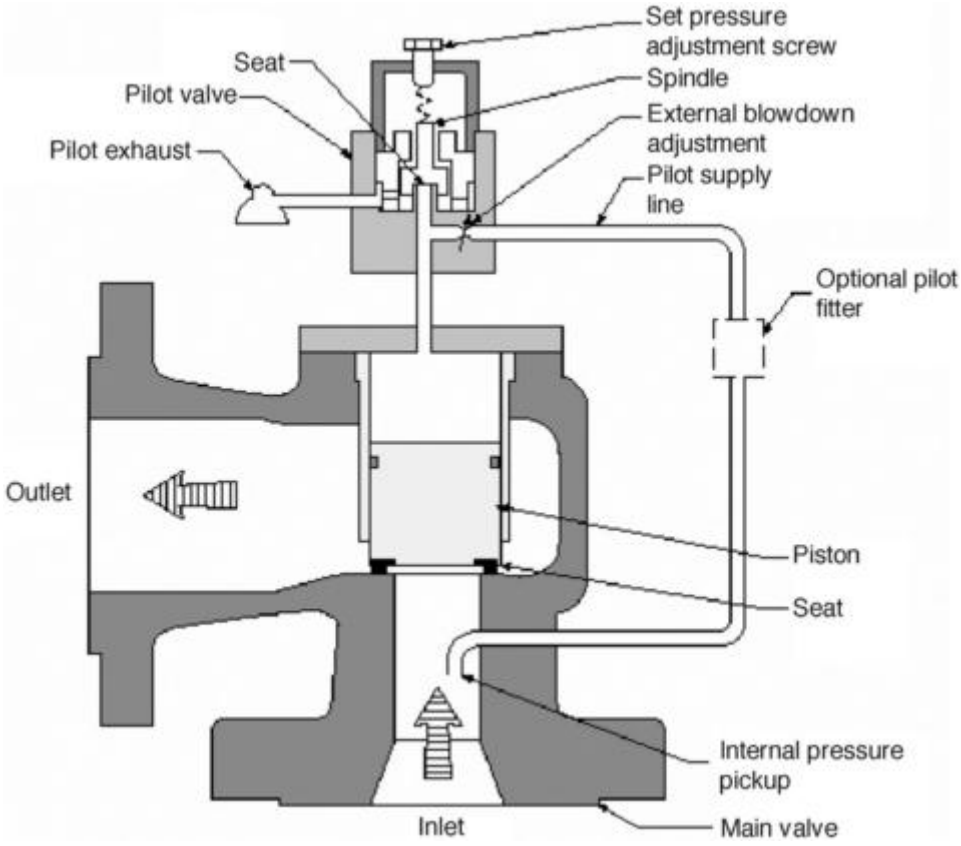


FIG. 10.13 Pop-action pilot-operated relief valve. *Reproduced with permission from API Recommended Practice 520.*

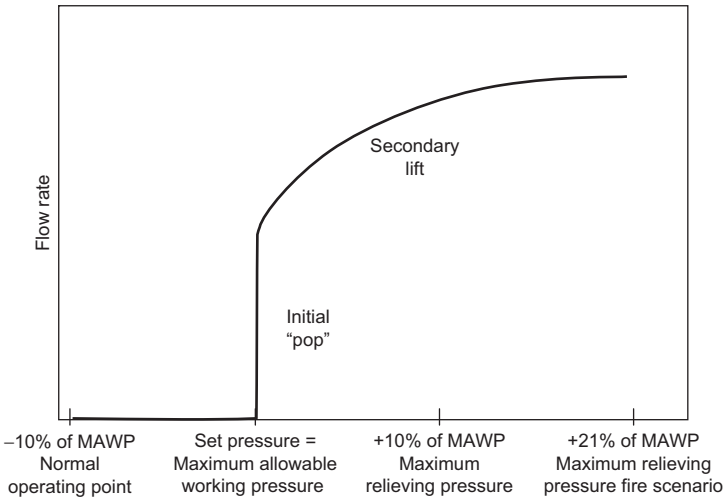


FIG. 10.14 Pressure–flow response of a pilot-operated relief valve.

When the fluid flowing through the valve is a compressible gas or a vapor, the design must consider whether critical flow is achieved in the nozzle of the valve. The critical flow rate is the maximum flow rate that can be achieved and corresponds to a sonic velocity at the nozzle. If critical flow occurs, the pressure at the nozzle exit cannot fall below the critical flow pressure P_{cf}, even if a lower pressure exists downstream. The critical flow pressure can be estimated from the upstream pressure for an ideal gas using the equation:

$$\frac{P_{cf}}{P_1} = \left[\frac{2}{\gamma+1}\right]^{\gamma/(\gamma-1)} \tag{10.18}$$

where γ = ratio of specific heats = C_p/C_v
P_1 = absolute pressure upstream
P_{cf} = critical flow pressure

Any consistent set of units may be used for pressure as long as the absolute pressure is used, not the gauge pressure. The ratio P_{cf}/P_1 is called the *critical pressure ratio*. Typical values of this ratio are given in Table 10.14. If the downstream pressure is less than the critical flow pressure, critical flow will occur in the nozzle. It can be seen from the table that this will be the case whenever the upstream pressure is more than two times the downstream pressure. Because most relief systems are operated close to atmospheric pressure, critical flow is the usual case.

For critical flow, API STD 520 (Section 3.6.2) gives the following equation for valve area, A_d:

$$A_d = \frac{13,160\ w}{C\ K_d\ P_1\ K_b\ K_c}\ \sqrt{\frac{T\ Z}{M_w}} \tag{10.19}$$

where A_d = discharge area, mm^2
w = required flow rate, kg/hr
C = coefficient = $520\sqrt{\gamma\left(\frac{2}{\gamma+1}\right)^{(\gamma\ +\ 1)/(\gamma\ -\ 1)}}$
K_d = coefficient of discharge
P_1 = absolute pressure upstream, kPa
K_b = back-pressure correction factor
K_c = combination correction factor

TABLE 10.14 Critical flow pressure ratios

Gas	Specific heat ratio $\gamma = C_p/C_v$ at 60 °F, 1 atm	Critical flow pressure ratio at 60 °F, 1 atm
Hydrogen	1.41	0.52
Air	1.40	0.53
Nitrogen	1.40	0.53
Steam	1.33	0.54
Ammonia	1.3	0.54
Carbon dioxide	1.29	0.55
Methane	1.31	0.54
Ethane	1.19	0.57
Ethylene	1.24	0.57
Propane	1.13	0.58
Propylene	1.15	0.58
n-Butane	1.19	0.59
n-Hexane	1.06	0.59
Benzene	1.12	0.58
n-Decane	1.03	0.60

Adapted from API RP 520.
Notes:
1. Taken from API RP 520, Table 7.
2. Some values of critical flow pressure ratio have been determined experimentally and do not necessarily agree with predictions from Equation 10.18.

T = relieving temperature, K
Z = compressibility at the inlet condition
M_w = molecular weight, g/mol

For preliminary estimates, the coefficient K_d can be taken as 0.975 for a relief valve and 0.62 for a bursting disk. The back-pressure correction factor, K_b, can initially be assumed to be 1.0 for critical flow. The combination correction factor, K_c, is used when a rupture disk is used upstream of the relief valve (see next section), in which case it is 0.9. If no rupture disk is used, then K_c, is 1.0. For vessels designed in accordance with ASME BPV Code Sec. VIII, $P_1 = 1.1$ times the maximum allowable working pressure.

The relief valve selected should be one with equal or greater area than calculated using Equation 10.19. Relief valve sizes are given in API STD 526 and BS EN ISO 4126. Sizing equations for subcritical flow of vapors, liquids, steam, and two-phase mixtures are given in API STD 520.

10.9.4 Design of non-reclosing pressure relief devices

Two types of non-reclosing pressure relief devices are used: rupture disks and breaking-pin devices.

A rupture disk device consists of a rupture disk and a clamp that holds the disk in position. The disk is made from a thin sheet of metal and is designed to burst if a set pressure is exceeded. Some rupture disks are scored so that they can burst without forming fragments that might damage downstream equipment.

Rupture disks are often used upstream of relief valves to protect the relief valve from corrosion or to reduce losses due to relief valve leakage. Large rupture disks are also used in situations that require very fast response time or high relieving load (for example, reactor runaway and external fire cases). They are also used in situations where pressure is intentionally reduced below the operating pressure for safety reasons. The use of bursting disk devices is described in BS EN ISO 4126-2 and BS EN ISO 4126-6.

If a rupture disk is used as the primary pressure-relief device, then when it bursts, the operators have no option but to shut down the plant so that the disk can be replaced before the vessel is repressured. Rupture disks are therefore most commonly used at the inlets of relief valves or as secondary relief devices. Rupture disks can be sized using Equation 10.19 for compressible gases in sonic flow, with a value of $K_d = 0.62$. The combination of safety valves and rupture discs is discussed in BS EN ISO 4126-3.

Breaking-pin devices have a similar construction to spring-loaded relief valves, except the valve disk is held against the seat by a pin that is designed to buckle or break when the set pressure is reached, as illustrated in Fig. 10.15. Once the valve has opened, the pin must be replaced before the valve can be reset.

Both rupture disks and breaking-pin devices are sensitive to temperature. The manufacturer should always be consulted for applications that are not at ambient conditions. Because non-reclosing pressure-relief devices can only be used once, the set pressure is determined by testing a sample of the devices out of each manufactured batch. Pressure-relief valve test methods are specified in ASME PTC 25.

10.9.5 Design of pressure-relief discharge systems

When designing relief venting systems, it is important to ensure that flammable or toxic gases are vented to a safe location. This will normally mean venting at a sufficient height to ensure that the gases are dispersed without creating a hazard. For highly toxic materials, it may be necessary to provide a scrubber to absorb and "kill" the material, for instance, the provision of caustic scrubbers for chlorine and hydrochloric acid gases. If flammable materials have to be vented at frequent intervals, as, for example, in some refinery operations, flare stacks are used.

The rate at which material can be vented will be determined by the design of the complete venting system: the relief device and the associated piping. The maximum venting rate will be limited by the critical (sonic) velocity, whatever the pressure drop. The vent system must be designed such that sonic flow can only occur at the relief valve and not elsewhere in the system; otherwise, the design relief load will not be attained. The design of venting systems to give adequate protection against overpressure is a complex and difficult subject, particularly if two-phase flow is likely to occur. When two-phase flow can occur, the relief system must provide for disengagement of liquid from the vapor before the vapor is vented or sent to flare.

Under normal closed conditions, the leakage from a properly designed and maintained spring-operated relief valve should be minimal; however, valves that open and close frequently or that are exposed to corrosive fluids or dust can suffer damage leading to increased leakage and may require more frequent inspection and maintenance. Leakage from relief valves can be a significant source of plant volatile organic compound (VOC) emissions if the

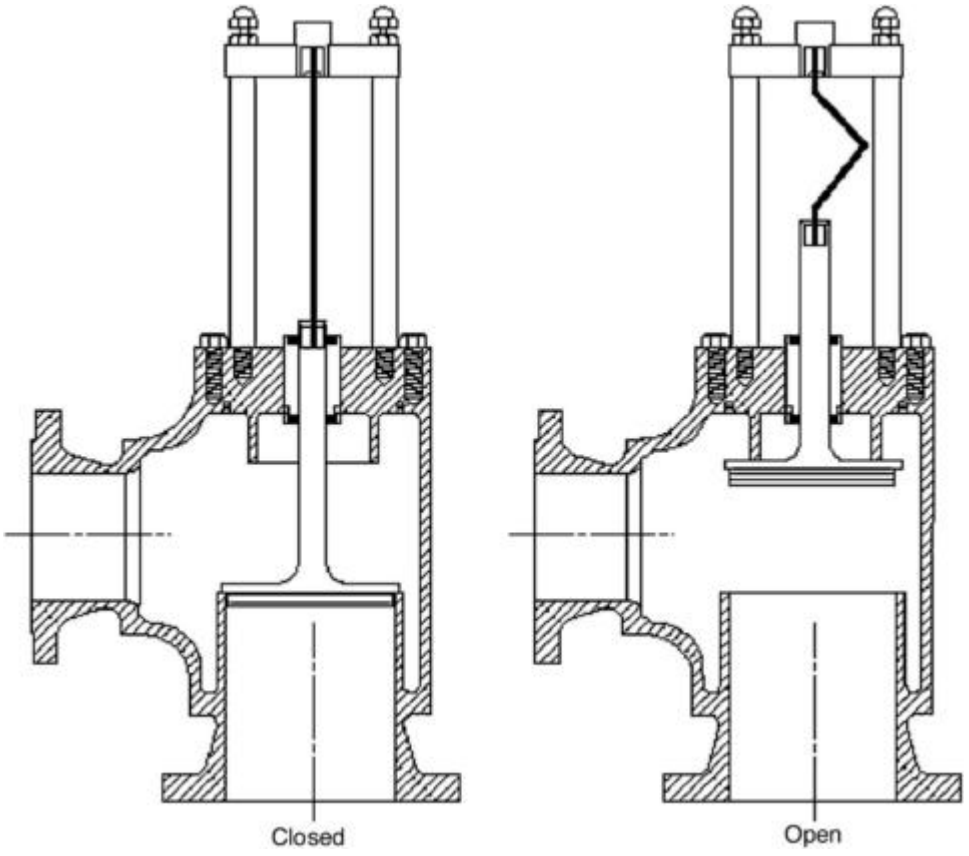


FIG. 10.15 Buckling-pin relief valve. *Reproduced with permission from API Recommended Practice 520.*

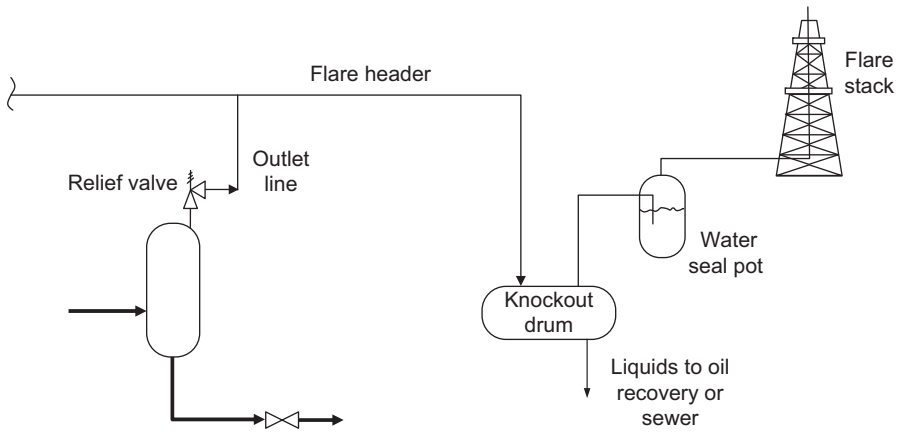


FIG. 10.16 Typical relief system design.

relief system does not vent via a flare stack. Methods for determining leakage from relief valves are given in API STD 527.

Guidelines for relief valve installation and relief systems design are given in API STD 520 Part II, API STD 521 Sections 4 and 5 and the DIERS Project Manual (Fisher et al., 1993). API STD 521 also gives design methods for blowdown drums and flare systems. A typical relief system is shown in Fig. 10.16. For a comprehensive discussion of the problem of vent system design and the design methods available, see the papers by Duxbury (1976, 1979) and the guidelines by CCPS (2017).

10.9.6 Protection from underpressure (vacuum)

Unless designed to withstand external pressure (see Section 14.7), a vessel must be protected against the hazard of underpressure, as well as overpressure. Underpressure will normally mean vacuum on the inside with atmospheric pressure on the outside. It requires only a slight drop in pressure below atmospheric pressure to collapse a storage tank. Though the pressure differential may be small, the force on the tank roof will be considerable. For example, if the pressure in a 10-m-diameter tank falls to 10 millibar below the external pressure, the total load on the tank roof will be around 80,000 N (equivalent to 8 metric tons weight). It is not an uncommon occurrence for a storage tank to be sucked in (collapsed) by the suction pulled by the discharge pump due to the tank vents having become blocked. Where practical, vacuum breakers (valves that open to atmosphere when the internal pressure drops below atmospheric) should be fitted.

Example 10.4

A gasoline surge drum has capacity 4 m^3 (1060 gal) and is normally operated 50% full at 40 °C (100 °F) under 20 bar absolute pressure (280 psig) of hydrogen in the head space and using a level controlled outflow, as shown in Fig. 10.10(a). Gasoline of specific gravity 0.7 is pumped into the surge drum at a normal flow rate of 130 m^3/hr.

Assuming the aspect ratio of the vessel (ratio length/diameter) is 3.0 and the heat of vaporization of gasoline is 180 BTU/lb, evaluate the relief loads for the blocked outflow and external fire cases and determine the relief valve size. (In practice, gasoline contains many components that boil over a wide range of temperatures at the design pressure, and a more complex calculation is needed than is given here.)

Blocked outlet case

$$w = \frac{1.1 P_m M_w v}{1000\, RT} = \frac{1.1 \times \left(\frac{130}{3600}\right) \times \left(\frac{20 \times 10^5}{0.9}\right) \times 2}{1000 \times 8.314 \times 313} = \underline{\underline{67.8 \text{ g/s}}} \tag{10.16}$$

External fire case

If the vessel has a hemispherical head, then:

$$\text{volume} = \pi \left(\frac{D^2 L}{4} + \frac{D^3}{6}\right) = \frac{11\pi D^3}{12}$$

$$\text{so } D = 1.12 \text{ m}$$

$$\text{wetted area} = \pi \left(DL + D^2\right)/2 = 2\pi D^2$$

$$= 7.82 \text{ m}^2 = 84.2 \text{ ft}^2$$

Assume $F_e = 1$:

$$w_f = \frac{21000\, F_e\, A_w^{0.82}}{\Delta H_{vap}} = \frac{21000 \times 1 \times 84.2^{0.82}}{180}$$

$$= 4423 \text{ lb/hr} \tag{10.17}$$

$$= \underline{\underline{0.56 \text{ kg/s}}}$$

So the external fire case has the higher relieving load and governs the design.

If the vent line discharges to a flare system at atmospheric pressure, then:

$$\frac{P_{outlet}}{P_1} = \frac{1}{20} << 0.52$$

so flow in the nozzle is critical.

For hydrogen:

$$C = 520\sqrt{1.41\left(\frac{2}{2.41}\right)^{(2.41/0.41))}}$$

$$= 356.9$$

Assume the valve will lift when the temperature reaches 60 °C (333K), $Z = 1.02$ for hydrogen:

$$A_d = \frac{13{,}160\ w}{C\ K_d\ P_1\ K_b\ K_c}\sqrt{\frac{TZ}{M_w}} = \frac{13160 \times 0.56 \times 3600}{356.9 \times 0.975 \times 2000 \times 1.0 \times 1.0}\sqrt{\frac{333 \times 1.02}{2}}$$

$$= 496.8\ \text{mm}^2 \text{ or } 0.77\ \text{in}^2 \tag{10.19}$$

From API STD 526, we would select an "H" orifice relief valve with effective orifice area 0.785 in^2. A size 2H3 carbon steel relief valve will allow a set pressure up to 740 psig in the expected range of operation temperature. In practice, however, we would have to consider two-phase flow due to entrainment of boiling liquid with the vapor and might select a larger orifice size after more detailed design.

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10.11 Nomenclature

		Dimensions in MLT
A_d	Discharge area	$\mathbf{L^2}$
A_w	Internal wetted surface area	$\mathbf{L^2}$
C	Impact of a hazard (impact per loss event) in Equation 10.1	
C	Constant in Equation 10.19	—
C_p	Specific heat capacity at constant pressure	$\mathbf{L^2T^{-2}\theta^{-1}}$
C_v	Specific heat capacity at constant volume	$\mathbf{L^2T^{-2}\theta^{-1}}$
D	Diameter	$\mathbf{L}$
F	Hazard rate (frequency of a hazard in events per year)	$\mathbf{T^{-1}}$
F_e	Environmental factor for external fire	—
F_{np}	Inherent frequency of a hazard with no protective system (number of events per year)	$\mathbf{T^{-1}}$
F_t	Tolerable frequency of a hazard (number of events per year)	$\mathbf{T^{-1}}$
F_3	Unit hazard factor in Dow Fire & Explosion Index	—
K_b	Back-pressure correction factor	—
K_c	Combination correction factor for a relief valve	—
K_d	Coefficient of discharge for a relief valve	—
L	Length of vessel	$\mathbf{L}$
M_w	Molecular weight	—
N_r	Reactivity in the Dow Fire & Explosion Index	—

		Dimensions in MLT
n	Number of moles of gas	**M**
P	Pressure	$\mathbf{ML^{-1}T^{-2}}$
P_{cf}	Critical flow pressure	$\mathbf{ML^{-1}T^{-2}}$
P_m	Maximum allowable working pressure	$\mathbf{ML^{-1}T^{-2}}$
P_1	Upstream pressure	$\mathbf{ML^{-1}T^{-2}}$
PFD_{av}	Average probability of failure on demand of a protective system	—
Q	Heat input due to fire	$\mathbf{ML^{2}T^{-3}}$
R	Ideal gas constant	$\mathbf{L^{2}T^{-2}\theta^{-1}}$
R_{np}	Inherent risk of a hazard with no protective system in place	
R_t	Tolerable risk, also sometimes called the *acceptable risk*	
T	Temperature	$\theta 1$
t	Time	**T**
V	Vessel volume	$\mathbf{L^{3}}$
V_G	Volume occupied by vapor	$\mathbf{L^{3}}$
V_L	Volume occupied by liquid	$\mathbf{L^{3}}$
v	Liquid volumetric flow rate	$\mathbf{L^{3}T^{-1}}$
w	Relieving mass flow rate	$\mathbf{MT^{-1}}$
w_f	Fire case relieving mass flow rate	$\mathbf{MT^{-1}}$
Z	Vapor compressibility	—
γ	Ratio of specific heat capacities	—
ΔH_{vap}	Heat of vaporization	$\mathbf{L^{2}T^{-2}}$
ΔR	Risk reduction factor, defined in Equation 10.3	
δ	Demand rate (number of occasions per year that a safety system is actuated)	$\mathbf{T^{-1}}$
Φ	Fractional dead time (probability that a safety system is inactive)	—
λ	Failure rate (number of occasions per year that a safety system develops a fault)	$\mathbf{T^{-1}}$
τ	Test interval	**T**

10.12 Problems

10.1. In the storage of flammable liquids, if the composition of the vapor–air mixture above the liquid surface falls within the flammability limits, a floating roof tank would be used or the tank blanketed with inert gas. Check if the vapor composition for liquids listed here will fall within their flammability range both at atmospheric pressure and 25 °C.
1. Toluene
2. Acrylonitrile
3. Nitrobenzene
4. Acetone

10.2. Complete a failure mode effects analysis for the nitric acid plant reactor section described in Example 10.2. (This is best carried out as a group activity with a group size of three to six.)

10.3. Estimate the Dow Fire and Explosion Index and determine the hazard rating for the processes listed here. Use the process descriptions given in Appendix F and develop the designs as needed to estimate the index.
1. Ethylhexanol from propylene and synthesis gas, F.1.
2. Chlorobenzenes from benzene and chlorine, F.2.
3. Methyl ethyl ketone from 2-butanol, F.3.
4. Acrylonitrile from propylene and ammonia, F.4.
5. Aniline from nitrobenzene and hydrogen. F.8.

10.4. Devise a preliminary control scheme for the sections of the nitric acid plant described in Chapter 2, flowsheet Fig. 2.8, which are listed here. Make a practice HAZOP study of each section and revise your preliminary control scheme.
1. Waste heat boiler (WHB)
2. Condenser
3. Absorption column

10.5. A distillation column separates benzene from toluene using a control scheme similar to that shown in Fig. 5.17(a). Make a practice HAZOP study of the plant section and add any instrumentation that is needed to develop the full P&I diagram.

10.6. Develop a fault tree for events that could lead to release of benzene to the atmosphere for the distillation section designed in Problem 10.5.

10.7. List the materials incompatibility problems you should be aware of in plants that handle:
1. Hydrogen peroxide
2. Ethylene oxide
3. Chlorine
4. Ammonium nitrate
5. Styrene

10.8. List possible relief scenarios for the vessel designed in Problem 14.1.

10.9. Estimate the relieving load for the reactor designed in Problem 14.5 for a blocked outlet scenario, and size the relief valve for this case.

10.10. A toluene surge drum has capacity 500 gal and is normally operated 60% full at 100 °F under 300 psig of hydrogen in the head space using a level controlled outflow. The normal flow rate into the vessel is 30,000 lb/hr. Determine the vessel dimensions if the vessel is vertically mounted. Evaluate the relief loads for the blocked outflow and external fire cases and determine the relief valve size.

CHAPTER

11

General site considerations

KEY LEARNING OBJECTIVES

- Factors that are considered in site selection and plant layout
- Environmental legislation that governs chemical plant operations
- Waste minimization methods that can be used to reduce the environmental impact of a chemical plant

11.1 Introduction

When a new chemical plant is being designed, one of the first decisions must be the plant location. If the project is for a new grassroots facility, a suitable site must be found and the site and equipment layout planned. If the plant is to go into an existing site, the impact on the existing infrastructure must be evaluated so that necessary modifications can be made to accommodate the new plant. In either case, provision must be made for the ancillary buildings and services needed for plant operation and for the environmentally acceptable disposal of effluent. These subjects are discussed briefly in this chapter.

11.2 Plant location and site selection

The location of the plant can have a crucial effect on the profitability of a project and the scope for future expansion. Many factors must be considered when selecting a suitable site, and only a brief review of the principal factors will be given in this section. Site selection for chemical process plants is discussed in more detail by Merims (1966) and Mecklenburgh (1985); see also CCPS (2003). The principal factors to consider are:

1. Location with respect to the marketing area
2. Raw material supply
3. Transport facilities
4. Availability of labor
5. Availability of utilities: water, fuel, and power
6. Availability of suitable land
7. Environmental impact, including effluent disposal
8. Local community considerations
9. Climate
10. Political, economic, and strategic considerations

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Marketing area

For materials that are produced in bulk quantities, such as cement, mineral acids, fuels, and fertilizers, where the cost of the product per metric ton is relatively low and the cost of transport is a significant fraction of the sales price, the plant should be located close to the primary market. This consideration is much less important for low-volume production, high-priced products, such as pharmaceuticals.

Raw materials

The availability and price of suitable raw materials will often determine the site location. Plants that produce bulk chemicals are best located close to the source of the major raw material, as long as the costs of shipping product are not greater than the cost of shipping feed. For example, at the time of writing much of the new ethylene capacity that is being added worldwide is being built in the Middle East, close to supplies of cheap ethane from natural gas. Oil refineries, on the other hand, tend to be located close to major population centers, as an oil refinery produces many grades of fuel, which are expensive to ship separately over long distances.

Transport

The transport of materials and products to and from the plant can be an overriding consideration in site selection. If practicable, a site should be selected that is close to at least two major forms of transport: road, rail, waterway (canal or river), or a sea port. Road transport is increasingly used, and is suitable for local distribution from a central warehouse. Rail transport is usually cheaper for the long-distance transport of bulk chemicals. Industrial gases and some bulk fuels are shipped by pipeline.

Air transport is convenient and efficient for the movement of personnel and essential equipment and supplies, and the proximity of the site to a major airport should be considered. Air freight can also be used for small volumes of high-value products such as pharmaceuticals, as long as the products are safe to transport by air and meet aviation regulations.

Availability of labor

Labor will be needed for construction of the plant and its operation. Skilled construction workers are often brought in from outside the site area, but there should be an adequate pool of unskilled labor available locally and labor suitable for training to operate the plant. Skilled craft workers such as electricians, welders, and pipe fitters will be needed for plant maintenance. Local labor laws, trade union customs, and restrictive practices must be considered when assessing the availability and suitability of the local labor for recruitment and training.

Utilities (services)

Chemical processes invariably require large quantities of water for cooling and general process use, and the plant must be located near a source of water of suitable quality. Process water may be drawn from a river, from wells, or purchased from a local supplier.

At some sites, cooling water can be taken from a river or lake or from the sea; at other locations cooling towers will be needed. In locations where the ambient humidity is high, use of cooling water may be unattractive compared with air cooling; see Section 3.2.5.

Electrical power is needed at all sites. Electrochemical processes (for example, chlorine manufacture or aluminum smelting) require large quantities of power and must be located close to a cheap source of power.

A competitively priced fuel must be available on site for steam and power generation.

Environmental impact and effluent disposal

All industrial processes produce waste products, and full consideration must be given to the difficulties and cost of their disposal. The disposal of toxic and harmful effluents will be covered by local regulations, and the appropriate authorities must be consulted during the initial site survey to determine the standards that must be met.

An environmental impact assessment should be made for each new project or major modification or addition to an existing process; see Section 11.5.6.

Local community considerations

The proposed plant must fit in with and be acceptable to the local community. Full consideration must be given to the safe location of the plant so that it does not impose a significant additional risk to the local population. Plants should generally be sited so as not to be upwind of residential areas under the prevailing wind.

On a new site, the local community must be able to provide adequate facilities for the plant personnel: schools, banks, housing, and recreational and cultural facilities.

The local community must also be consulted about plant water consumption and discharge and the effect of the plant on local traffic. Some communities welcome new plant construction as a source of new jobs and economic prosperity. More affluent communities generally do less to encourage the building of new manufacturing plants, and in some cases may actively oppose chemical plant construction.

Land (site considerations)

Sufficient suitable land must be available for the proposed plant and for future expansion. The land should ideally be flat, well drained, and have suitable load-bearing characteristics. A full site evaluation should be made to determine the need for piling or other special foundations. Particular care must be taken when building plants on reclaimed land near the ocean in earthquake zones because of the poor seismic character of such land.

Climate

Adverse climatic conditions at a site will increase costs. Abnormally low temperatures require the provision of additional insulation and special heating for equipment and pipe runs. Stronger structures are needed at locations subject to high winds (cyclone/hurricane areas) or earthquakes.

Political and strategic considerations

Capital grants, tax concessions, and other inducements are often given by governments to direct new investment to preferred locations, such as areas of high unemployment. The availability of such grants can be the overriding consideration in site selection.

In a globalized economy, there may be an advantage to be gained by locating the plant within an area with preferential tariff agreements, such as the European Union (EU).

Corporations make strategic decisions on plant location, for example, trading off the desire to satisfy the needs of emerging markets against the risk of locating capital assets in countries that do not have strong enforcement of intellectual property rights. These factors are discussed in more detail in Section 9.9.

11.3 Site layout

The process units and ancillary buildings should be laid out to give the most economical flow of materials and personnel around the site. Hazardous processes must be located at a safe distance from other buildings. Consideration must also be given to the future expansion of the site. The ancillary buildings and services required on a site, in addition to the main processing units (buildings), include:

1. Storage for raw materials and products: tank farms and warehouses
2. Shipping and receiving areas: road or rail tanker filling and unloading facilities, truck loading
3. Maintenance workshops
4. Stores for maintenance and operating supplies
5. Laboratories for process quality control
6. Fire stations and other emergency services
7. Utilities: steam boilers, compressed air, power generation, refrigeration, transformer stations
8. Effluent disposal plant: waste water treatment, solid and or liquid waste collection
9. Offices for general administration
10. Canteens and other amenity buildings, such as medical centers
11. Parking lots

When roughing out the preliminary site layout, the process units are normally sited first and arranged to give a smooth flow of materials through the various processing steps, from receiving of raw material to final product storage and shipping. Process units are normally spaced at least 30 m apart; greater spacing may be needed for hazardous processes.

The location of the principal ancillary buildings should then be decided. They should be arranged so as to minimize the time spent by personnel traveling between buildings. Administration offices and laboratories, in which a relatively large number of people will be working, should be located well away from potentially hazardous

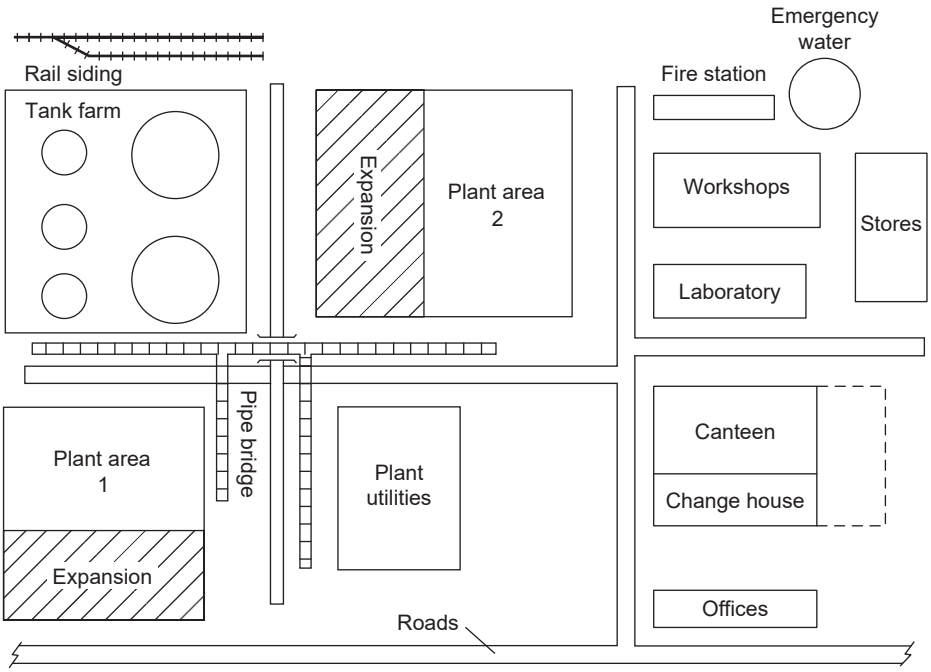


FIG. 11.1 Typical site plan.

processes. Control rooms are normally located adjacent to the processing units, but with potentially hazardous processes may have to be sited at a safer distance.

The siting of the main process units determines the layout of the plant roads, pipe alleys, and drains. Access roads to each building are needed for construction and for operation and maintenance.

Utility buildings should be sited to give the most economical run of pipes to and from the process units.

Cooling towers should be sited so that under the prevailing wind the plume of condensate spray drifts away from the plant area and adjacent properties.

The main storage areas should be placed between the loading and unloading facilities and the process units they serve. Storage tanks containing hazardous materials should be sited at least 70 m (200 ft) from the site boundary.

A typical plot plan is shown in Fig. 11.1.

A comprehensive discussion of site layout is given by Mecklenburgh (1985); see also House (1969), Kaess (1970), and Meissner and Shelton (1992).

11.4 Plant layout

The economic construction and efficient operation of a process unit will depend on how well the plant and equipment specified on the process flowsheet is laid out.

A detailed account of plant layout techniques cannot be given in this short section. A fuller discussion can be found in the book edited by Mecklenburgh (1985) and in articles by Kern (1977a–f, 1978a–f), Meissner and Shelton (1992), Brandt et al. (1992), and Russo and Tortorella (1992).

The principal factors to be considered are:

1. Economic considerations: construction and operating costs
2. The process requirements
3. Convenience of operation
4. Convenience of maintenance
5. Safety
6. Future expansion
7. Modular construction

Costs

The cost of construction can be minimized by adopting a layout that gives the shortest run of connecting pipe between equipment and the least amount of structural steel work; however, this will not necessarily be the best arrangement for operation and maintenance.

Process requirements

An example of the need to take into account process considerations is the need to elevate the base of columns to provide the necessary net positive suction head to a pump (see Chapter 20) or the operating head for a thermosiphon reboiler (see Chapter 19).

Operation

Equipment that needs to have frequent operator attention should be located convenient to the control room. Valves and instruments should be located at convenient positions and heights for operator access. Sample points must be convenient for operator access and must also be near to a drain point so that sample lines can be flushed. Sufficient working space and headroom must be provided to allow easy access to equipment. If it is anticipated that equipment will need replacement, then sufficient space must be allowed to permit access for lifting equipment.

Maintenance

Heat exchangers need to be sited so that the tube bundles can be easily withdrawn for cleaning and tube replacement. Vessels that require frequent replacement of catalyst or packing should be located on the outside of buildings. Equipment that requires dismantling for maintenance, such as compressors and large pumps, should be placed under cover.

Safety

Blast walls may be needed to isolate potentially hazardous equipment and confine the effects of an explosion. At least two escape routes for operators must be provided from each level in process buildings.

Plant expansion

Equipment should be located so that it can be conveniently tied in with any future expansion of the process.

Space should be left on pipe racks for future needs, and service pipes should be oversized to allow for future requirements.

Modular construction

In recent years there has been a move to assemble sections of plant at the plant manufacturer's site. These modules include the equipment, structural steel, piping, and instrumentation. The modules are then transported to the plant site by road or by sea.

The advantages of modular construction are:

1. Improved quality control
2. Reduced construction cost
3. Less need for skilled labor on site
4. Less need for skilled personnel on overseas sites

Some of the disadvantages are:

1. Higher design costs
2. More structural steel work
3. More flanged connections
4. Possible problems with on-site assembly

A fuller discussion of techniques and applications of modular construction is given by Shelley (1990), Hesler (1990), and Whittaker (1984).

General considerations

Open structural steelwork buildings are normally used for process equipment. Closed buildings are used for process operations that require protection from the weather, for small plants, or for processes that require ventilation with scrubbing of the vent gas.

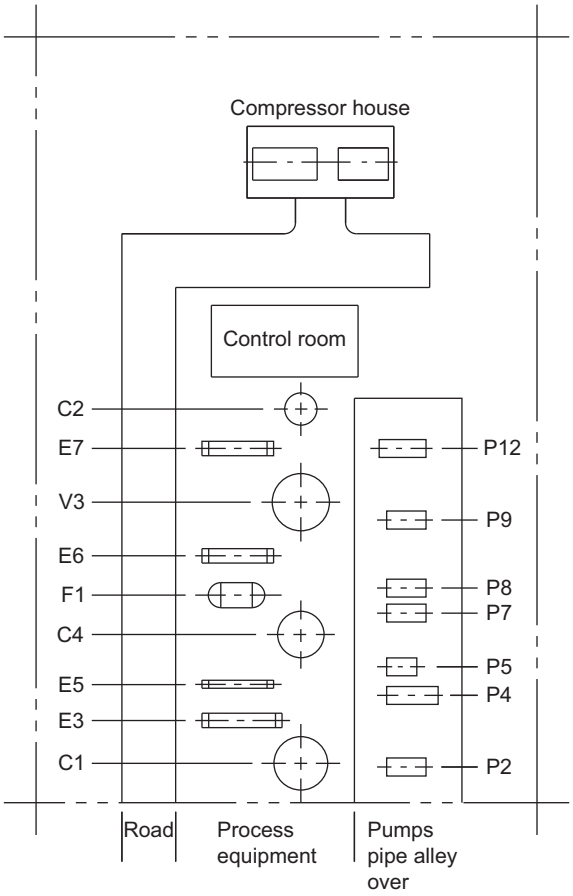


FIG. 11.2 A typical plant layout.

The arrangement of the major items of equipment often follows the sequence given on the process flowsheet, with the columns and vessels arranged in rows and the ancillary equipment, such as heat exchangers and pumps, positioned along the outside. A typical preliminary layout is shown in Fig. 11.2.

11.4.1 Techniques used in site and plant layout

Cardboard cutouts of the equipment outlines can be used to make trial plant layouts. Simple models, made up from rectangular and cylindrical blocks, can be used to study alternative layouts in plan and elevation. Cutouts and simple block models can also be used for site layout studies. Once the layout of the major pieces of equipment has been decided, the plan and elevation drawings can be made and the design of the structural steelwork and foundations undertaken.

Large-scale models, to a scale of at least 1:30, are sometimes still made for major projects. These models are used for piping design and to decide the detailed arrangement of small items of equipment, such as valves, instruments, and sample points. Piping isometric diagrams can be taken from the finished models. The models are also useful on the construction site and for operator training. Proprietary kits of parts are available for the construction of plant models.

Computer-aided design (CAD) tools are being increasingly used for plant layout studies, and computer models are complementing, if not yet completely replacing, physical models. Several proprietary programs are available for the generation of three-dimensional models of plant layout and piping. Present systems allow designers to zoom in on a section of plant and view it from various angles. Developments of computer technology will soon enable engineers to virtually walk through the plant. A typical computer-generated model is shown in Fig. 11.3.

Some of the advantages of computer graphics modeling compared with actual scale models are:

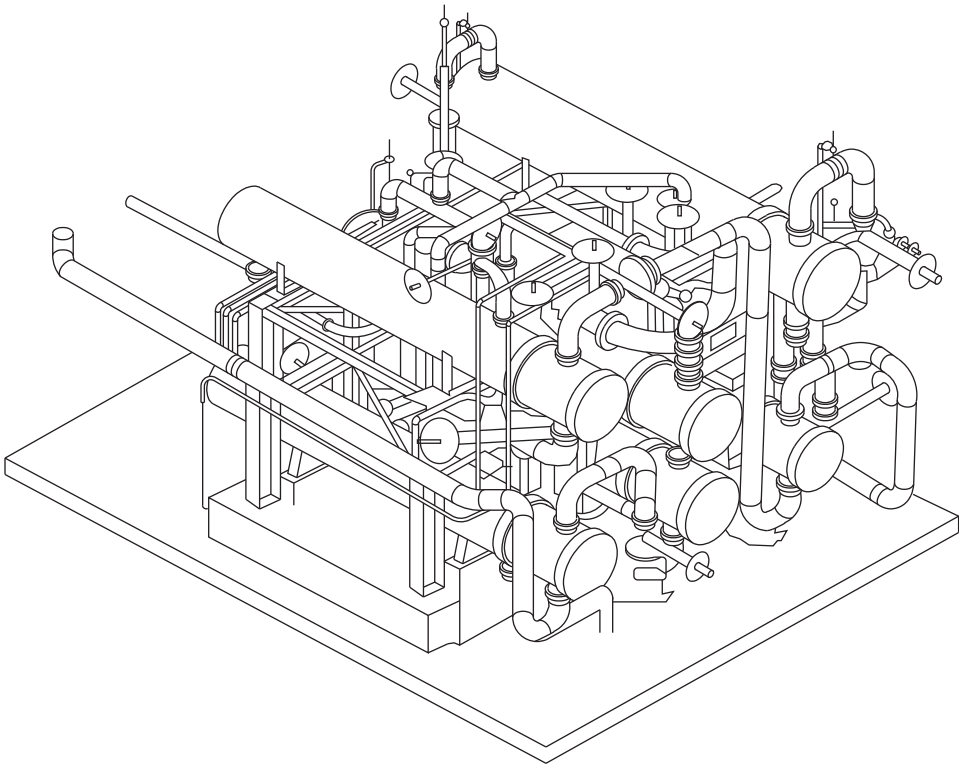


FIG. 11.3 Computer-generated layout "model." *Courtesy: Babcock Construction Ltd.*

1. The ease of electronic transfer of information. Piping drawings can be generated directly from the layout model. Bills of quantities: materials, valves, instruments, etc., are generated automatically.
2. The computer model can be part of an integrated project information system, covering all aspects of the project from conception to operation.
3. It is easy to detect interference between pipe runs, and pipes and structural steel that occupy the same space.
4. The physical model has to be transported to the plant site for use in the plant construction and operator training. A computer model can be instantly available in the design office, the customer's offices, and at the plant site.
5. Expert systems and optimization programs can be incorporated in the package to assist the designer to find the best practical layout; see Madden et al. (1990).

11.5 Environmental considerations

All individuals and companies have a duty of care to their neighbors and to the environment in general. In addition to this moral duty, most countries have enacted strict laws to protect the environment and preserve the quality of air, water, and land.

Vigilance is required in both the design and operation of process plants to ensure that legal standards are met and that no harm is done to the environment.

Consideration must be given to:

1. All emissions to land, air, and water
2. Waste management
3. Smells
4. Noise
5. Visual impact
6. Any other nuisances
7. The environmental friendliness of the products

11.5.1 Environmental legislation

It is not feasible to review the entire body of legislation that has been enacted to protect the environment in this chapter. States, provinces, and municipalities often pass local legislation that is stricter than the national laws. For example, the South Coast Air Quality Management District (SCAQMD), which sets air quality standards for the Los Angeles basin, has consistently advocated air quality limits that exceed the U.S. national standards. The interpretation of statutes can change over time as a result of court decisions and executive orders, and environmental legislation is also revised frequently, so the design engineer should always check with the local, regional, and federal authorities to ensure that the correct standards are being applied in the design and to ensure that the correct information is being generated for permit applications. This section provides a brief overview of some of the main environmental laws in North America. More information on U.S. federal laws can be found on the U.S. Environmental Protection Agency (EPA) website at www.epa.gov/laws-regulations. Information on Canadian laws is given on the Environment Canada website at www.canada.ca/en/environment-climate-change. Full citations for all of the laws are given in the references in Section 11.6.

The National Environmental Policy Act of 1969

The National Environmental Policy Act (NEPA) requires that all legislation must consider environmental impact. Government agencies must prepare environmental impact assessments. The president must make an annual Environmental Quality Report to Congress, discussing current status and recent trends in the air, water, and terrestrial environments; natural resources; and government programs that have impacts on the environment.

The act also established the Council on Environmental Quality in the Executive Office of the President, with goals of assisting in the preparation of the Environmental Quality Report, reviewing government programs, carrying out research, and recommending national policies to improve environmental protection.

The Clean Air Act (1970)

The Clean Air Act (CAA) was enacted to improve air quality. The CAA was amended and strengthened in 1990. Under the CAA, the EPA is empowered to set National Ambient Air Quality Standards (NAAQS), which are allowable ambient levels for seven contaminants:

1. Ozone
2. Carbon monoxide
3. Lead
4. Nitrogen dioxide
5. Sulfur dioxide
6. PM10: particulate matter with mean diameter less than 10 μm
7. PM2.5: particulate matter with mean diameter less than 2.5 μm

Areas that fail to meet the NAAQS levels are classified as "nonattainment" areas and must take remediation steps, such as mandating the use of cleaner-burning, federal reformulated gasoline.

The CAA also mandated the EPA to set the U.S. National Emission Standards for Hazardous Air Pollutants (NESHAP). These standards regulate air emissions of 189 listed hazardous air pollutants. The standards were set based on the best 12% of controlled facilities in each industry. A similarly high technical standard was set by EPA in the Maximum Available Control Technology rules (MACT) that have been applied to emissions of volatile organics (1995) and sulfur and other inorganic compounds (2002) from oil refineries.

The CAA has had a significant impact on ambient levels of the pollutants that it regulates. Acid precipitation and surface water acidity have been reduced, particularly in the Midwest and Northeast. Ozone nonattainment has not been so successful, as ozone formation is closely linked to emissions of nitrogen oxides, which are not as tightly regulated. Charts showing nonattainment regions can be downloaded from www.epa.gov.

The Federal Water Pollution Control Act ("The Clean Water Act," 1972)

The initial goal of the Clean Water Act (CWA) was to achieve clean water for swimming, boating, and protecting fish and wildlife by 1983. The act was amended in 1977 and 1987 to strengthen the focus on water quality and emissions of toxic compounds.

The CWA empowers the EPA to set water quality standards for pollutants in surface waters. Under the CWA, effluent guidelines are established for each industrial sector. It is unlawful to discharge any pollutant into navigable waters without a permit from the EPA.

The Safe Drinking Water Act (1974)

The Safe Drinking Water Act (SDWA) authorized the EPA to set standards on the required purity of surface or subterranean water that could potentially be used for drinking. Owners and operators of public water systems must comply with these EPA standards. The SDWA established the Office of Ground Water and Drinking Water (OGDW) to oversee implementation of the act and protect public health by ensuring safe drinking water.

The Resource Conservation and Recovery Act (1976)

The ultimate goal of the Resource Conservation and Recovery Act (RCRA) is to protect groundwater from contamination. The legislation addresses only current and future facilities, as abandoned or historic sites are covered by CERCLA and SARA, described later.

Under RCRA, waste producers are required to take a "cradle to grave" approach to waste management. The producer of the waste is legally liable from the moment that waste is produced until its final disposal. A waste generator must identify waste material as "hazardous waste" if it is on a regulatory list or has a characteristic of flammability, toxicity, corrosivity, or reactivity. Once a material has been identified as hazardous waste, it must be clearly labeled and tracked when in transport. The waste must be treated in special facilities to low levels of contaminants. The final residual solid material, for example, incinerator ash, must be disposed into a registered hazardous waste landfill.

Additional regulations to aid in the identification of hazardous waste are given in the Code of Federal Regulations (40 CFR 261.3, 1999).

The Comprehensive Environmental Response, Compensation and Liability Act (or Superfund, 1980)

The Superfund act addressed hazardous waste from abandoned operations and historic production sites. The act created a tax on the chemical and petroleum industries to pay for remediation of uncontrolled or abandoned hazardous waste sites. Prohibitions and other requirements were established for abandoned sites, including liability for anyone responsible for a release of hazardous material at such a site.

The Comprehensive Environmental Response, Compensation and Liability Act (CERCLA) legislation also authorized the EPA to take action to remediate sites, either by short-term removal of material if there was an immediate threat of release or longer-term remediation actions if there was no immediate threat to life.

The Superfund Amendments and Reauthorization Act (1986)

The Superfund Amendments and Reauthorization Act (SARA) of 1986 amended CERCLA and made additions to the program. The act stressed the importance of permanent remediation and the use of innovative cleanup technologies. Greater participation of citizens, local communities, and state governments in all steps of the Superfund program was encouraged. The EPA was required to revise the Hazard Ranking System (HRS) to ensure that it accurately assessed the relative degree of risk to human health and the environment caused by uncontrolled hazardous waste sites. The size of the trust fund for site restoration was increased to $8.5 billion. Title III of SARA authorized the Emergency Planning and Community Right-to-Know Act (EPCRA) cited in Chapter 10.

The Pollution Prevention Act (1990)

The Pollution Prevention Act (PPA) was passed to encourage waste minimization and reduction of pollution at the source by more efficient processing and raw materials use. The EPA was authorized to promote source reduction and recycling through grants, technical assistance, and dissemination of information.

The Oil Pollution Act of 1990 (1990)

The Oil Pollution Act (OPA) was passed in the aftermath of the Exxon Valdez oil spill in the Prince William Sound in Alaska. It created a tax on oil to cover the cost of responding to major spills when the responsible party is unwilling or unable to do so. The limits on liability for causing oil spills are clearly laid out in the law, and oil shippers and storage facilities are required to submit plans for responding to a large spill to the EPA.

The major environmental laws in Canada are discussed next.

The Department of the Environment Act (E-10, 1985)

This act established the Department of the Environment and defined the responsibilities of the Minister of the Environment. The minister was charged with establishing programs to protect the environment and reduce pollution, ensuring that new federal programs are assessed for environmental impact, and reporting environmental information to the Canadian public.

The Canadian Environmental Protection Act (C-33, 1999)

The Canadian Environmental Protection Act (CEPA) charges Environment Canada with controlling toxic substances, reducing pollution, and eliminating persistent bio-accumulating toxic substances. Enforcement officers are given the power to issue environmental protection compliance orders on the spot to stop illegal activity and correct any violations of the act.

CEPA is also the preferred legislation that Canada will use to enforce regulations to meet its commitments to reduce greenhouse gas emissions as a signatory of the Kyoto Protocol.

The Canada Water Act (C-11, 1985)

The Canada Water Act empowers the Minister of the Environment to conclude agreements with the provinces on water resource management and water quality management. Drinking water and recreational water quality standards are set by Health Canada.

11.5.2 Waste minimization

Waste arises mainly as by-products or unused reactants from the process, or as off-specification product produced through misoperation. There will also be fugitive emissions from leaking seals and flanges and inadvertent spills and discharges through misoperation. In emergency situations, material may be discharged to the atmosphere through vents normally protected by bursting disks and relief valves.

Before considering "end-of-pipe" approaches for treating and managing waste products, the design engineer should always try to minimize production of waste at the source. The hierarchy of waste management approaches is:

1. Source reduction: Don't make the waste in the first place. This is the best practice.
2. Recycle: Find a use for the waste stream.
3. Treatment: Reduce the severity of the environmental impact.
4. Disposal: Meet the requirements of the law.

Source reduction is accomplished during process design. Some of the strategies that can be considered include:

1. *Purification of feeds.* Reducing the concentration of impurities in the feed usually leads to reduced side reactions and less waste formation. This approach can also reduce the need for purges and vent streams. Feed impurities also often lead to degradation of solvents and catalysts. Care must be taken to select a purification approach that does not itself lead to more waste formation.
2. *Protect catalysts and adsorbents.* Deactivated catalysts and adsorbents are solid wastes from the process. In some cases, relatively small amounts of contaminants can cause a load of catalyst or adsorbent to become useless. The catalyst or adsorbent should be protected by using a guard bed of suitable material to adsorb or filter out contaminants before they can damage the catalyst.
3. *Eliminate use of extraneous materials.* When different solvent or mass separating agents are used, this leads to waste formation when the solvents become degraded. If the plant or site uses relatively few solvents, it may be economical to build a solvent-recovery plant. Liquid wastes from spent solvents are common in fine chemicals and pharmaceuticals manufacture.
4. *Increase recovery from separations.* Higher product recovery leads to lower concentrations of product in the waste streams. Higher purity recycle streams usually lead to less waste formation. These benefits must always be traded off against the extra capital and energy costs involved in driving the separation processes to higher recovery or purity.
5. *Improve fuel quality.* Switching to a cleaner-burning fuel, such as natural gas, reduces the emissions from fired heaters. In some locations this must be traded off against the higher cost of natural gas relative to heating oil and coal.

Unused reactants can be recycled and off-specification product reprocessed. Integrated processes can be selected, with the waste from one process becoming the raw material for another. For example, the otherwise waste hydrogen chloride produced in a chlorination process can be used for chlorination using a different reaction, as in the balanced, chlorination-oxyhydrochlorination process for vinyl chloride production. It may be possible to sell waste to another company for use as raw material in their manufacturing processes, for example, the use of off-specification and recycled plastics in the production of lower-grade products, such as the ubiquitous black plastic bucket.

Processes and equipment should be designed to reduce the chances of misoperation by providing tight control systems, alarms, and interlocks. Sample points, process equipment drains, and pumps should be sited so that any leaks flow into the plant effluent collection system, not directly to sewers. Hold-up systems, tanks, and ponds should be provided to retain spills for treatment. Flanged joints should be kept to the minimum needed for the assembly and maintenance of equipment. Fugitive emissions from packings and seals can be reduced by specifying dual seals, dry-gas seals, or seal-less pumps.

A technique that is sometimes used for waste minimization is the five-step review:

1. Identify waste *components* for regulatory impact.
2. Identify *waste streams* for size and economic impact.
3. List the *root causes* of the waste streams.
4. List and analyze *modifications* to address the root causes.
5. Prioritize and *implement* the best solutions.

The information gathered in the first two steps is often collected in an effluent summary worksheet. An effluent summary lists the regulated pollutants produced by the process and summarizes the quantities produced and where they originate. The effluent summary can be used to focus waste minimization efforts and as a basis for the design of effluent treatment processes. The information in the effluent summary may also be required for obtaining permits to operate the plant or for preparing more formal environmental impact analyses to convince investors or insurers that environmental impact has been properly addressed. An example effluent summary sheet is given in Appendix G. A template is available in Microsoft Excel format in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

The American Petroleum Institute Publication 302 (1991) discusses source reduction, recycle, treatment, and disposal of wastes. Other source reduction techniques are given by Smith and Petela (1991) and El-Halwagi (2017). The UK Institution of Chemical Engineers has published a guide to waste minimization (IChemE 1997).

11.5.3 Waste management

When waste is produced, processes must be incorporated in the design for its treatment and safe disposal. The following techniques can be considered:

1. Dilution and dispersion
2. Discharge to foul-water sewer (with the agreement of the appropriate authority)
3. Physical treatments: scrubbing, settling, absorption, and adsorption; see Chapter 16
4. Chemical treatment: precipitation (for example, of heavy metals), neutralization
5. Biological treatment: activated sludge and other processes
6. Incineration on land or at sea
7. Landfill at controlled sites
8. Sea dumping (now subject to tight international control)

Several standards have been written to address waste management systems. In the United States, EPA standard 40 CFR 260 (2006) provides general guidelines, while EPA 40 CFR 264 (2006) gives standards for waste treatment, storage, and disposal. Standards for the petroleum industry are given in API publications 300 (1991) and 303 (1992). The main international standard for waste management systems is ISO 140001 (2004), which has been adopted as the national standard in the countries of the EU. ASTM standard 11.04 (2006) should also be consulted.

Gaseous wastes

Gaseous effluents that contain toxic or noxious substances need treatment before discharge into the atmosphere. The practice of relying on dispersion from tall stacks is seldom entirely satisfactory. Gaseous pollutants can be removed by absorption or adsorption. Absorption by scrubbing with water or a suitable solvent or base is probably the most widely used method for high-volume gas streams, while adsorption onto activated carbon or a zeolitic adsorbent is used for smaller gas streams. The design of adsorption plants is addressed in Chapter 16, and the design of scrubbing towers is described in Chapter 17. Finely dispersed solids can be removed by scrubbing or using electrostatic precipitators; see Chapter 18. Flammable gases can be burnt. The sources of air pollution and their control are covered in several books: Walk et al. (1997), Heumann (1997), Davies (2000), Cooper and Ally (2010), and Schnelle et al. (2017). McGowan and Santoleri (2007) discuss methods for reducing emissions of volatile organic compounds (VOCs).

Liquid wastes

The waste liquids from a chemical process, other than aqueous effluent, will usually be flammable and can be disposed of by burning in suitably designed incinerators. Care must be taken to ensure that the temperatures attained in the incinerator are high enough to completely destroy any harmful compounds that may be formed, such as the possible formation of dioxins when burning chlorinated compounds. The gases leaving an incinerator may be scrubbed and acid gases neutralized. A typical incinerator for burning gaseous or liquid wastes is shown in Chapter 3, Fig. 3.13. The design of incinerators for hazardous waste and the problems inherent in the disposal of waste by incineration are discussed by Butcher (1990) and Baker-Counsell (1987).

In the past, small quantities of liquid waste in drums were disposed of by dumping at sea or in landfill sites. This is not an environmentally acceptable method and is now subject to stringent controls.

Solid wastes

Solid waste can be burnt in suitable incinerators or disposed by burial at licensed landfill sites. As with liquid wastes, the dumping of toxic solid waste at sea is no longer acceptable.

Aqueous wastes

Aqueous waste streams include process water, utility wastewater, and site run-off. Water that is used or formed in the process must be sent to effluent treatment. Common process water effluents include:

- Water contaminated with ammonia or hydrogen sulfide from gas scrubbers
- Salt waters from deionizers, softeners, neutralization steps, and washing operations
- Water contaminated with hydrocarbons, for example, from condensers
- Biologically contaminated water, for example, fermentation broths or water from washing operations
- Spent acid and caustic streams

The site utility systems produce large wastewater flows. A purge known as a ”blowdown” is taken from both the cooling water and the boiler feed water to prevent the accumulation of solids in either recirculating system. Cooling water blowdown is often the largest contributor to the site wastewater. The blowdown streams can be high in minerals content and also contain chemicals such as biocides and corrosion inhibitors that have been added to the boiler feed water or cooling water.

It is also a best practice to collect run-off water from the plant area and treat it in the site wastewater plant before discharging it to the environment. Run-off water can come from rain, fire hydrant flushing, and equipment washing. As the water flows over the ground around the plant, it can become contaminated with organic chemicals that have leaked from the plant. Most plants are designed so that all the run-off is collected into local sewers or ditches that are routed to the site wastewater treatment plant.

The principal factors that determine the nature of an aqueous industrial effluent and on which strict controls will be placed by the responsible authority are:

1. pH
2. Suspended solids
3. Toxicity
4. Biological oxygen demand

The pH can be adjusted by the addition of acid or alkali. Spent acid or alkali solutions must usually be neutralized before they can be sent to water treatment plants. Lime (calcium oxide) is frequently used to neutralize acidic effluents. In the case of sulfuric acid, the use of lime leads to formation of calcium sulfate. Calcium sulfate that is potentially contaminated with trace organic material has low value and can be used as road fill. An alternative approach is to neutralize with more expensive ammonia, forming ammonium sulfate, which can be sold as a fertilizer.

Suspended solids can be removed by settling, using clarifiers (see Chapter 18).

For some effluents, it is possible to reduce the toxicity to acceptable levels by dilution. Other effluents need chemical treatment.

The oxygen concentration in a water course must be maintained at a level sufficient to support aquatic life. For this reason, the biological oxygen demand of an effluent is of utmost importance. It is measured by a standard test: the BOD5 (5-day biological oxygen demand). This test measures the quantity of oxygen that a given volume of the effluent (when diluted with water containing suitable bacteria, essential inorganic salts, and saturated with oxygen) will absorb in 5 days, at a constant temperature of 20 °C. The results are reported as parts of oxygen

absorbed per million parts effluent (ppm). The BOD5 test is a rough measure of the strength of the effluent: the organic matter present. It does not measure the total oxygen demand, as any nitrogen compounds present will not be completely oxidized in 5 days. The ultimate oxygen demand (UOD) can be determined by conducting the test over a longer period, up to 90 days. If the chemical composition of the effluent is known, or can be predicted from the process flow-sheet, the UOD can be estimated by assuming complete oxidation of the carbon present to carbon dioxide and the nitrogen present to nitrate:

$$\mathrm{UOD} = 2.67\mathrm{C} + 4.57\mathrm{N}$$

where C and N are the concentrations of carbon and nitrogen in ppm by weight.

Activated sludge processes are usually used to reduce the biological oxygen demand of an aqueous effluent before discharge. Where wastewater is discharged into the sewers with the agreement of the local water authorities, a charge will normally be made according to the BOD value and any treatment required. Where treated effluent is discharged to water courses with the agreement of the appropriate regulatory authority, the BOD5 limit will typically be set at 20 ppm. A full discussion of aqueous effluent treatment is given by Eckenfelder et al. (1985); see also Eckenfelder (1999).

11.5.4 Noise

Noise can cause a serious nuisance in the neighborhood of a process plant. Care must be taken when selecting and specifying equipment such as compressors, air-cooler fans, induced and forced draught fans for furnaces, conveyors, grinders, dryers, and other noisy plant. Excessive noise can also be generated when venting through steam and other relief valves and from flare stacks. Such equipment should be fitted with silencers. Vendors' specifications should be checked to ensure that equipment complies with statutory noise levels, both for the protection of employees (see Chapter 10) and for noise pollution considerations. Noisy equipment should, as far as practicable, be sited well away from the site boundary. Earth banks and screens of trees can be used to reduce the noise level perceived outside the site.

11.5.5 Visual impact

The appearance of the plant should be considered at the design stage. There is little that can be done to change the appearance of a modern-style plant, where most of the equipment and piping are outside and in full view, but some steps can be taken to minimize the visual impact. Large equipment, such as storage tanks, can be painted to blend in with, or even contrast with, the surroundings. For example, the Richmond oil refinery in the San Francisco Bay Area has its storage tanks painted to blend in with the surrounding hills. Landscaping and screening by belts of trees can also help improve the overall appearance of the site.

11.5.6 Environmental auditing

An environmental audit is a systematic examination of how a business operation affects the environment. It will include all emissions to air, land, and water and cover the legal constraints, the effect on the community, the landscape, and the ecology. Products will be considered, as well as processes. When applied at the design stage of a new development, it is more correctly called an *environmental impact assessment*.

The aims of the audit or assessment are to:

1. Identify environmental problems associated with manufacturing process and the use of the products before they become liabilities
2. Develop standards for good working practices
3. Provide a basis for company policy
4. Ensure compliance with environmental legislation
5. Satisfy requirements of insurers
6. Be seen to be concerned with environmental questions, which is important for public relations
7. Minimize the production of waste, which is an economic factor

Environmental auditing is discussed in the books by Grayson (1992), McGaw (1993), and Pain (2018).

Life cycle assessment

Life cycle assessment is a more exhaustive procedure than environmental auditing and is used to compare the long-term sustainability of alternative designs. A life cycle assessment considers all the environmental costs and impacts of the process, its feed stocks, and the physical plant itself, from initial construction through to final decommissioning and site remediation. The methods for carrying out a life cycle assessment are given in ISO standards BS EN ISO 14040 and BS EN ISO 14044 (which have superseded the older 14041, 14042, and 14043 standards). A good introduction to life cycle assessment is given by Clift (2001). Many examples of life cycle assessments can be found in the journals *Environmental Science and Technology*, *Environmental Progress*, and *The International Journal of Life Cycle Assessment*.

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CHAPTER

12

Optimization in design

KEY LEARNING OBJECTIVES

- How to improve a design using optimization methods
- Understand the role of constraints in limiting designs
- How to recognize design trade-offs
- Awareness of the methods used for solving optimization problems
- Why experienced design engineers very rarely use rigorous optimization methods in industrial practice

12.1 Introduction

Optimization is an intrinsic part of design: the designer seeks the best, or optimum, solution to a problem.

Many design decisions can be made without formally setting up and solving a mathematical optimization problem. The design engineer will often rely on a combination of experience and judgment, and in some cases the best design will be immediately obvious. Other design decisions have such a trivial impact on process costs that it makes more sense to make a close guess at the answer than to properly set up and solve the optimization problem. In every design, though, there will be several problems that require more rigorous optimization. This chapter introduces the techniques for formulating and solving optimization problems, as well as some of the pitfalls that are commonly encountered in optimization.

In this book, the discussion of optimization will, of necessity, be limited to a brief overview of the main techniques used in process and equipment design. Chemical engineers working in industry use optimization methods for process operations far more than they do for design, as discussed in Section 12.12. Chemical engineering students would benefit greatly from more classes in operations research methods, which are generally part of the industrial engineering curriculum. These methods are used in almost every industry for planning, scheduling, and supply chain management, all of which are critical operations for plant operation and management. There is an extensive literature on operations research methods and several good books on the application of optimization methods in chemical engineering design and operations. A good overview of operations research methods is given in the classic introductory text by Hillier and Lieberman (2014). Applications of optimization methods in chemical engineering are discussed by Rudd and Watson (1968), Stoecker (1989), Floudas (1995), Biegler et al. (1997), Edgar and Himmelblau (2001), and Diwekar (2008).

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12.2 The design objective

An optimization problem is always stated as the maximization or minimization of a quantity called the objective. For chemical engineering design projects, the objective should be a measure of how effectively the design meets the customer's needs. This will usually be a measure of economic performance. Some typical objectives are given in Table 12.1.

The overall corporate objective is usually to maximize operating income, cash flow, or earnings before interest and taxes (EBIT), but the design engineer will often find it more convenient to use other objectives when working on subcomponents of the design. The optimization of subsystems is discussed in more detail in Section 12.5.

The first step in formulating the optimization problem is to state the objective as a function of a finite set of variables, sometimes referred to as the decision variables:

$$z = f(x_1,\ x_2,\ x_3,\ \ldots,\ x_n) \tag{12.1}$$

where:

z = objective
$x_1, x_2, x_3, \ldots, x_n$ = decision variables

This function is called the objective function. The decision variables may be independent, but they will usually be related to each other by many constraint equations. The optimization problem can then be stated as a maximization or minimization of the objective function subject to the set of constraints. Constraint equations are discussed in the next section.

Design engineers often face difficulties in formulating the objective function. Some of the economic objectives that are widely used in making investment decisions lead to intrinsically difficult optimization problems. For example, discounted cash flow rate of return (DCFROR) is difficult to express as a simple function and is highly nonlinear, whereas net present value (NPV) increases with project size and is unbounded unless a constraint is set on plant size or available capital. Optimization is therefore often carried out using simple objectives such as "minimize cost of production."

Health, safety, environmental, and societal impact costs and benefits are difficult to quantify and relate to economic benefit. These factors can be introduced as constraints, but few engineers would advocate building a plant in which every piece of equipment was designed for the minimum legally permissible safety and environmental performance. An experienced designer would usually select a design that was marginally worse in economic performance if it was clearly significantly safer.

An additional complication in formulating the objective function is the quantification of uncertainty. Economic objective functions are generally highly sensitive to the prices used for feeds, raw materials, and energy and to estimates of project capital cost. These costs and prices are forecasts or estimates and are usually subject to substantial error. Cost estimation and price forecasting are discussed in Chapters 7 and 8. There may also be uncertainty in the decision variables, either from variation in the plant inputs, variations introduced by unsteady plant operation, or imprecision in the design data and the constraint equations. Optimization under uncertainty is a specialized subject in its own right and is beyond the scope of this book. See Chapter 5 of Diwekar (2008) for a good introduction to the subject.

TABLE 12.1 Typical design optimization objectives

Maximize	Minimize
Project net present value	Project expense
Return on investment	Cost of production
Reactor productivity per unit volume	Total annualized cost
Plant availability (time on stream)	Plant inventory (for safety reasons)
Process yield of main product	Formation of waste products

12.3 Constraints and degrees of freedom

12.3.1 Constraints

The constraints on the optimization are the set of equations that bound the decision variables and relate them to each other.

If we write $\mathbf{x}$ as a vector of n decision variables, then we can state the optimization problem as:

$$\begin{aligned} &\text{Optimize (Max. or Min.) } z = f(\mathbf{x}) \\ &\text{subject to (s.t.):} \quad \mathbf{g}(\mathbf{x}) \leq 0 \\ &\qquad\qquad\qquad\quad \mathbf{h}(\mathbf{x}) = 0 \end{aligned} \tag{12.2}$$

where: z = the scalar objective
$f(\mathbf{x})$ = the objective function
$\mathbf{g}(\mathbf{x})$ = a m_i vector of inequality constraints
$\mathbf{h}(\mathbf{x})$ = a m_e vector of equality constraints
The total number of constraints is $m = m_i + m_e$

Equality constraints arise from conservation equations (mass, mole, energy, and momentum balances) and constitutive relations (the laws of chemistry and physics, correlations of experimental data, design equations, etc.). Any equation that is introduced into the optimization model that contains an "=" sign will become an equality constraint. Many examples of such equations can be found throughout this book.

Inequality constraints generally arise from the external constraints discussed in Section 1.2: safety limits, legal limits, market and economic limits, technical limits set by design codes and standards, feed and product specifications, availability of resources, etc. Some examples of inequality constraints might include:

Main product purity $\geq$ 99.99 wt%
Feed water concentration $\leq$ 20 ppmw
NO_x emissions $\leq$ 50 kg/yr
Production rate $\leq$ 400,000 metric tons per year
Maximum design temperature for ASME Boiler and Pressure Vessel Code Section VIII Division 2 $\leq$ 900 °F
Investment capital $\leq$ $50 MM (50 million dollars)

The effect of constraints is to limit the parameter space. This can be illustrated using a simple two-parameter problem:

$$\begin{aligned} &\text{Max.} \quad z = {x_1}^2 + 2{x_2}^2 \\ &\text{s.t.} \quad x_1 + x_2 = 5 \\ &\qquad\quad x_2 \leq 3 \end{aligned}$$

The two constraints can be plotted on a graph of x_1 vs. x_2, as in Fig. 12.1.

In the case of this example, it is clear by inspection that the set of constraints does not bound the problem. In the limit $x_1 \to \infty$, the solution to the equality constraint is $x_2 \to -\infty$, and the objective function gives $z \to \infty$, so no maximum can be found. Problems of this kind are referred to as unbounded. For this problem to have a solution, we need an additional constraint of the form:

$$\begin{aligned} &x_1 \leq \text{a (where a} > 2) \\ &x_2 \geq \text{b (where b} < 3) \\ \text{or} \quad &h(x_1, x_2) = 0 \end{aligned}$$

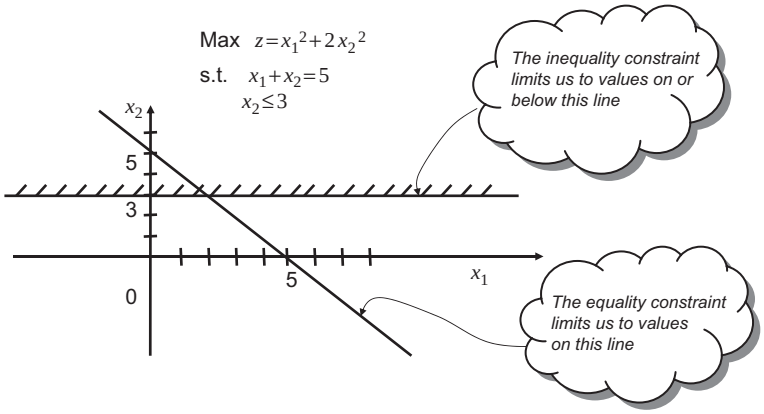


FIG. 12.1 Constraints on a simple optimization problem.

to define a closed search space.

It is also possible to overconstrain the problem. For example, if we set the problem:

$$\text{Max.} \quad z = x_1^2 + 2x_2^2$$

$$\text{s.t.} \quad x_1 + x_2 = 5$$

$$x_2 \leq 3$$

$$x_1 \leq 1$$

In this case, it can be seen from Fig. 12.2 that the feasible region defined by the inequality constraints does not contain any solution to the equality constraint. The problem is therefore infeasible as stated.

12.3.2 Degrees of freedom

If the problem has n variables and m_e equality constraints, then it has $n - m_e$ degrees of freedom. If $n = m_e$ then there are no degrees of freedom and the set of m_e equations can be solved for the n variables. If $m_e > n$ then the problem is over-specified. In most cases, however, $m_e < n$ and $n - m_e$ is the number of parameters that can be independently adjusted to find the optimum.

When inequality constraints are introduced into the problem, they generally set bounds on the range over which parameters can be varied and hence reduce the space in which the search for the optimum is carried out. Very often, the optimum solution to a constrained problem is found to be at the edge of the search space (i.e., at one of the inequality constraint boundaries). In such cases, that inequality constraint becomes equal to zero (as written in Equation 12.2) and is said to be *active*. It is often possible to use engineering insight and understanding of chemistry and physics to simplify the optimization problem. If the behavior of a system is well understood, the design engineer can

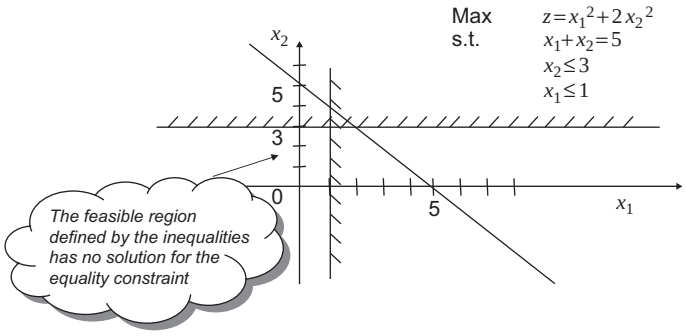


FIG. 12.2 An overconstrained problem.

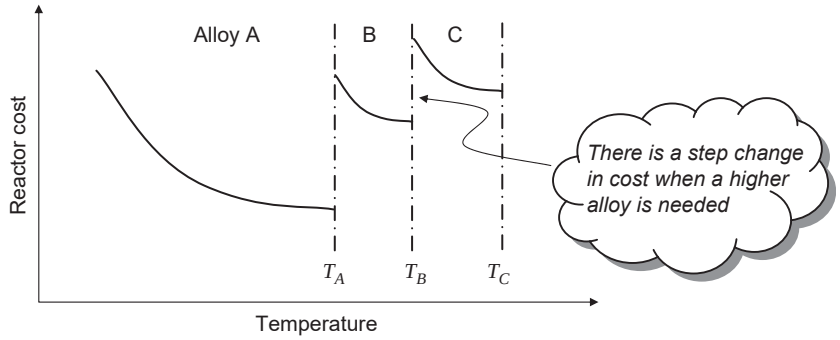


FIG. 12.3 Variation of reactor cost with temperature.

decide that an inequality constraint is likely to be active. By converting the inequality constraint into an equality constraint, the number of degrees of freedom is reduced by one and the problem is made simpler.

This can be illustrated by a simple reactor optimization example. The size and cost of a reactor are proportional to residence time, which decreases as temperature is increased. The optimal temperature is usually a trade-off between reactor cost and the formation of by-products in side reactions. But if there were no side reactions, then the next constraint would be the maximum temperature allowed by the pressure vessel design code. More expensive alloys might allow for operation at higher temperatures. The variation of reactor cost with temperature will look something like Fig. 12.3, where T_A, T_B, and T_C are the maximum temperatures allowed by the vessel design code for alloys A, B, and C, respectively.

The design engineer could formulate this problem in several ways. It could be solved as three separate problems, one corresponding to each alloy, each with a constraint on temperature $T < T_{alloy}$. The design engineer would then pick the solution that gave the best value of the objective function. The problem could also be formulated as a mixed-integer, nonlinear program with integer variables to determine the selection of alloy and set the appropriate constraint (see Section 12.11). The design engineer could also recognize that alloy A costs a lot less than alloy B, and the higher alloys only give a relatively small extension in the allowable temperature range. It is clear that cost decreases with temperature, so the optimum temperature will be T_A for alloy A and T_B for alloy B. Unless the design engineer is aware of some other effect that has an impact on cost as temperature is increased, it is safe to write $T = T_A$ as an equality constraint and solve the resulting problem. If the cost of alloy B is not excessive, then it would be prudent to also solve the problem with $T = T_B$, using the cost of alloy B.

The correct formulation of constraints is the most important step in setting up an optimization problem. Inexperienced engineers are often unaware of many constraints and consequently find "optimal" designs that are dismissed as unfeasible by more experienced designers.

12.4 Trade-offs

If the optimal value of the objective is not at a constraint limit, it will usually be determined by a trade-off between two or more effects. Trade-offs are common in design, because better performance in terms of increased purity, increased recovery, or reduced energy or raw materials use usually comes at the expense of higher capital expense, operating expense, or both. The optimization problem must capture the trade-off between cost and benefit.

A well-known example of a trade-off is the optimization of process heat recovery. A high degree of heat recovery requires close temperature approaches in the heat exchangers (see Section 3.5), which leads to high capital cost as the exchangers require more surface area. If the minimum temperature approach is increased, the capital cost is reduced but less energy is recovered. We can plot the capital cost and energy cost against the minimum approach temperature, as shown schematically in Fig. 12.4. If the capital cost is annualized (see Section 9.7) then the two costs can be added to give a total cost. The optimum value of the approach temperature, $\Delta T_{optimum}$, is then given by the minimum point in the total cost curve.

Some common trade-offs encountered in the design of chemical plants include:

- More separations equipment and operating cost vs. lower product purity
- More recycle costs vs. increased feed use and waste formation

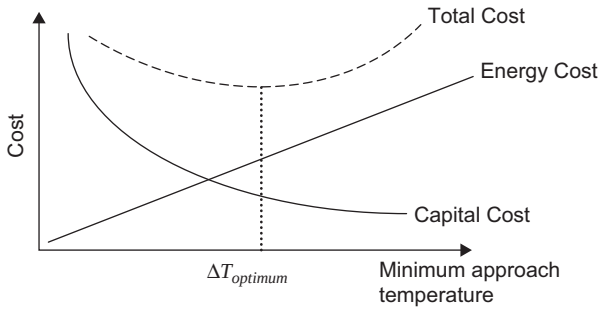


FIG. 12.4 The capital–energy trade-off in process heat recovery.

- More heat recovery vs. cheaper heat exchange network
- Higher reactivity at high pressure vs. more expensive reactors and higher compression costs
- Fast reactions at high temperature vs. product degradation
- Marketable by-products vs. more plant expense
- Cheaper steam and electricity vs. more off-site capital cost

Stating an optimization problem as a trade-off between two effects is often useful in conceptualizing the problem and interpreting the optimal solution. For example, in the case of process heat recovery, it is usually found that the shape of the total cost curve in Fig. 12.4 is relatively flat over the range 15 °C $< \Delta T_{optimum} <$ 40 °C. Knowing this, most experienced designers would not worry about finding the value of $\Delta T_{optimum}$, but would instead select a value for the minimum temperature approach within the range 15 °C to 40 °C, based on knowledge of the customer's preference for high energy efficiency or low capital expense.

12.5 Problem decomposition

The task of formally optimizing the design of a complex processing plant involving several hundred variables, usually with highly nonlinear relationships between the variables, is formidable, if not impossible. The task can be reduced by dividing the process into more manageable units, identifying the key variables, and concentrating work where the effort will give the greatest benefit. Some caution is needed when optimizing subproblems.

Subdivision, and optimization of the subunits rather than the whole, will not necessarily give the optimum design for the whole process. The optimization of one unit may be at the expense of another. For example, it will usually be satisfactory to optimize the reflux ratio for a distillation column independently of the rest of the plant, but if the column is part of a separation stage following a reactor, in which the product is separated from the unreacted materials, then the design of the column will interact with, and may well determine, the optimization of the reactor design. Care must always be taken to ensure that subcomponents are not optimized at the expense of other parts of the plant.

Equipment optimization is usually treated as a subproblem that is solved after the main process variables such as reactor conversion, recycle ratios, and product recoveries have been optimized. For example, the detailed design of heat exchangers is usually a trade-off between pressure drop and heat transfer. Higher shell- or tube-side velocities will give a higher heat-transfer coefficient, leading to a lower area and cheaper exchanger, but will also cause a higher pressure drop. A common practice is to make an allowance for exchanger pressure drop when solving the process flowsheet and then optimize the heat exchanger design subject to not exceeding the constraint of allowable pressure drop during detailed design. If heat exchanger costs are a significant fraction of total capital cost, this approach can lead to poor overall optimization, as the arbitrary assignment of pressure drops and inaccurate estimation of heat transfer coefficients in the process-level model will probably not lead to the optimal design.

Another example of a problem decomposition that is often applied is the use of the pinch design method in heat exchanger network design, described in Sections 3.5.1 and 3.5.3. If we choose to follow the pinch design rule, then no heat should be transferred across the pinch, and the heat exchanger network design problem is decomposed into two separate, smaller problems above and below the pinch. This is convenient, particularly when solving relatively small problems as hand calculations. Unfortunately, this approach has the drawback that we might miss opportunities to match the same streams above and below the pinch and hence reduce the number of exchangers needed by combining an exchanger from the above-pinch problem with one from the below-pinch problem. When designing

large networks involving many process streams and multiple utility streams, the imposition of utility pinches, as well as process pinches, can lead to the formation of impractical networks with many small heat exchangers.

12.6 Optimization of a single decision variable

If the objective is a function of a single variable, x, the objective function $f(x)$ can be differentiated with respect to x to give $f'(x)$. Any stationary points in $f(x)$ can then be found as the solutions of $f'(x) = 0$. If the second derivative of the objective function is greater than zero at a stationary point, then the stationary point is a local minimum. If the second derivative is less than zero, then the stationary point is a local maximum, and if it is equal to zero, then it is a saddle point. If x is bounded by constraints, then we must also check the values of the objective function at the upper and lower limiting constraints. Similarly, if $f(x)$ is discontinuous, then the value of $f(x)$ on either side of the discontinuity should also be checked.

This procedure can be summarized as the following algorithm:

$$\begin{aligned} \text{Min.} \quad & z = f(x) \\ \text{s.t.} \quad & x \geq x_L \\ & x \leq x_U \end{aligned} \tag{12.3}$$

1. Solve $f' = \frac{df(x)}{dx} = 0$ to find values of x_S.
2. Evaluate $f'' = \frac{d^2f(x)}{dx^2}$ for each value of x_S. If $f'' > 0$ then x_S corresponds to a local minimum in $f(x)$.
3. Evaluate $f(x_S)$, $f(x_L)$, and $f(x_U)$.
4. If the objective function is discontinuous, then evaluate $f(x)$ on either side of the discontinuity, x_{D1} and x_{D2}.
5. The overall optimum is the value from the set (x_L, x_S, x_{D1}, x_{D2}, x_U) that gives the lowest value of $f(x)$.

This is illustrated graphically in Fig. 12.5(a) for a continuous objective function. In Fig. 12.5(a), x_L is the optimum point, even though there is a local minimum at x_{S1}. Fig. 12.5(b) illustrates the case of a discontinuous objective function. Discontinuous functions are quite common in engineering design, arising, for example, when changes in temperature or pH cause a change in metallurgy. In Fig. 12.5(b) the optimum is at x_{D1}, even though there is a local minimum at x_S.

If the objective function can be expressed as a differentiable equation, then it is usually also easy to plot a graph like those in Fig. 12.5 and quickly determine whether the optimum lies at a stationary point or a constraint.

12.7 Search methods

In design problems, the objective function very often cannot be written as a simple equation that is easily differentiated. This is particularly true when the objective function requires solving large computer models, possibly using several different programs and requiring several minutes, hours, or days to converge a single solution. In such cases, the optimum is found using a search method. The concept of search methods is most easily explained for single-variable problems, but search methods are at the core of the solution algorithms for multivariable optimization as well.

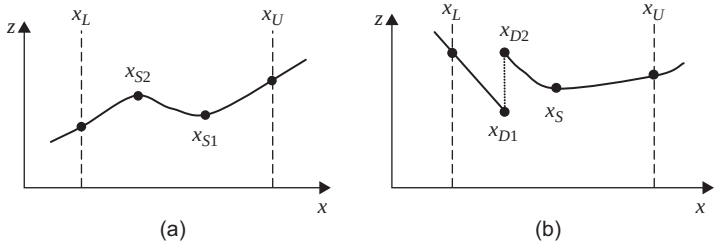


FIG. 12.5 Optimization of a single variable between bounds.

12.7.1 Unrestricted search

If the decision variable is not bounded by constraints, then the first step is to determine a range in which the optimum lies. In an unrestricted search, we make an initial guess of x and assume a step size, h. We then calculate $z_1 = f(x)$, $z_2 = f(x + h)$, and $z_3 = f(x - h)$. From the values of z_1, z_2, and z_3 we determine the direction of search that leads to improvement in the value of the objective, depending on whether we wish to minimize or maximize z. We then continue increasing (or decreasing) x by successive steps of h until the optimum is passed.

In some cases, it may be desirable to accelerate the search procedure, in which case the step size can be doubled at each step. This gives the sequence $f(x + h)$, $f(x + 3h)$, $f(x + 7h)$, $f(x + 15h)$, etc.

Unrestricted searching is a relatively simple method of bounding the optimum for problems that are not constrained. In engineering design problems, it is almost always possible to state upper and lower bounds for every parameter, so unrestricted search methods are not widely used in design.

Once a restricted range that contains the optimum has been established, restricted range search methods can be used. These can be broadly classified as direct methods that find the optimum by eliminating regions in which it does not lie and indirect methods that find the optimum by making an approximate estimate of $f'(x)$.

12.7.2 Regular search (three-point interval search)

The three-point interval search starts by evaluating $f(x)$ at the upper and lower bounds, x_L and x_U, and at the center point $(x_L + x_U)/2$. Two new points are then added in the midpoints between the bounds and the center point, at $(3x_L + x_U)/4$ and $(x_L + 3x_U)/4$, as shown in Fig. 12.6. The three adjacent points with the lowest values of $f(x)$ (or the highest values for a maximization problem) are then used to define the next search range.

By eliminating two of the four quarters of the range at each step, this procedure reduces the range by half each cycle. To reduce the range to a fraction ε of the initial range therefore takes n cycles, where $\varepsilon = 0.5^n$. Because each cycle requires calculating $f(x)$ for two additional points, the total number of calculations is $2n = 2 \log \varepsilon / \log 0.5$.

The procedure is terminated when the range has been reduced sufficiently to give the desired precision in the optimum. For design problems, it is usually not necessary to specify the optimal value of the decision variables to high precision, so ε is usually not a very small number.

12.7.3 Golden-section search

The golden-section search, sometimes called the golden mean search, is as simple to implement as the regular search but is more computationally efficient if $\varepsilon < 0.29$. In the golden-section search only one new point is added at each cycle.

The golden-section method is illustrated in Fig. 12.7. We start by evaluating $f(x_L)$ and $f(x_U)$ corresponding to the upper and lower bounds of the range, labeled A and B in the figure. We then add two new points, labeled C and D, each located a distance ωAB from the bounds A and B, that is, located at $x_L + \omega(x_U - x_L)$ and $x_U - \omega(x_U - x_L)$. For a minimization problem, the point that gives the highest value of $f(x)$ is eliminated. In Fig. 12.7, this is point B. A single new point, E, is added, such that the new set of points $AECD$ is symmetric with the old set of points $ACDB$.

For the new set of points to be symmetric with the old set of points, $AE = CD = \omega AD$.

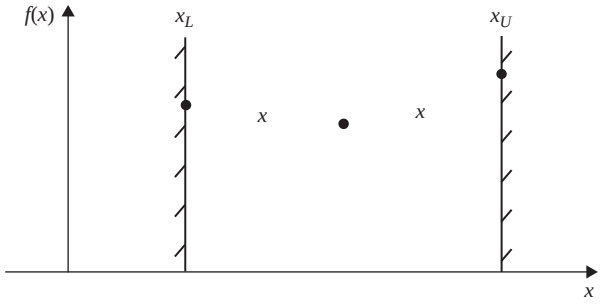


FIG. 12.6 Regular search.

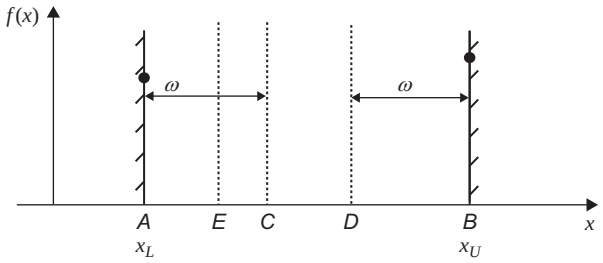


FIG. 12.7 Golden section search.

But we know $DB = \omega AB$, so $AD = (1 - \omega)AB$ and $CD = (1 - 2\omega)AB$
so $(1 - 2\omega) = \omega(1 - \omega)$

$$\omega = \frac{3 \pm \sqrt{5}}{2}$$

Each new point reduces the range to a fraction $(1 - \omega) = 0.618$ of the original range. To reduce the range to a fraction ε of the initial range therefore requires $n = \log \varepsilon / \log 0.618$ function evaluations.

The number $(1 - \omega)$ is known as the *golden mean*. The significance of this number has been known since ancient times. Livio (2002) gives a very entertaining account of its history and occurrence in art, architecture, music, and nature.

12.7.4 Quasi-Newton method

Newton's method is a super-linear, indirect search method that seeks the optimum by solving $f'(x)$ and $f''(x)$ and searching for where $f'(x) = 0$. The value of x at step $k + 1$ is calculated from the value of x at step k using:

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)} \tag{12.4}$$

and the procedure is repeated until $(x_{k+1} - x_k)$ is less than a convergence criterion or tolerance, ε.

If we do not have explicit formulae for $f'(x)$ and $f''(x)$, then we can make a finite difference approximation about a point, in which case:

$$x_{k+1} = x_k - \frac{[f(x_k + h) - f(x_k - h)]/2h}{[f(x_k + h) - 2f(x) + f(x_k - h)]/h^2} \tag{12.5}$$

Care is needed in setting the step size, h, and the tolerance for convergence, ε. The quasi-Newton method generally gives fast convergence unless $f''(x)$ is close to zero, in which case convergence is poor.

All of the methods discussed in this section are best suited for unimodal functions, that is, functions with no more than one maximum or minimum within the bounded range.

12.8 Optimization of two or more decision variables

A two-variable optimization problem can be stated as:

$$\begin{aligned} \text{Min.} \quad & z = f(x_1, x_2) \\ \text{s.t.} \quad & h(x_1, x_2) = 0 \\ & g(x_1, x_2) \leq 0 \end{aligned} \tag{12.6}$$

For simplicity, all problems will be stated as minimization problems from here on. A maximization problem can be rewritten as Min. $z = -f(x_1, x_2)$.

With two parameters, we can plot contour lines of z on a graph of x_1 vs. x_2 and hence get a visual representation of the behavior of z. For example, Fig. 12.8 shows a schematic of a contour plot for a function that exhibits a local minimum of <30 at about (4,13) and a global minimum of <10 at about (15,19). Contour plots are useful for understanding some of the key features of multivariable optimization that become apparent as soon as we consider more than one decision variable.

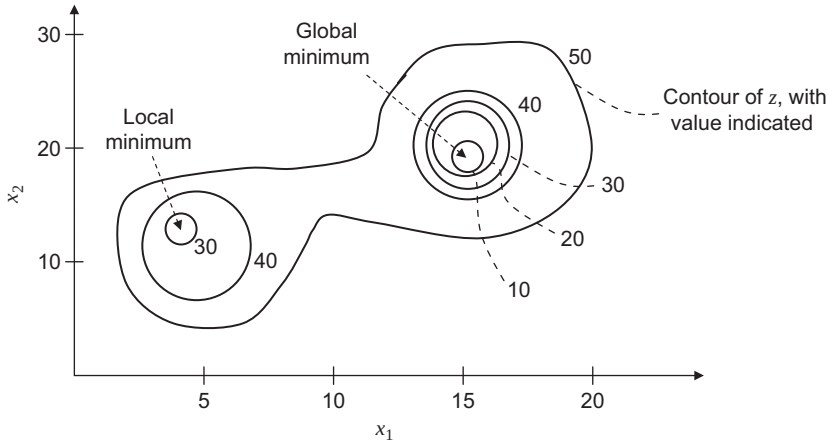


FIG. 12.8 Optimization of two decision variables.

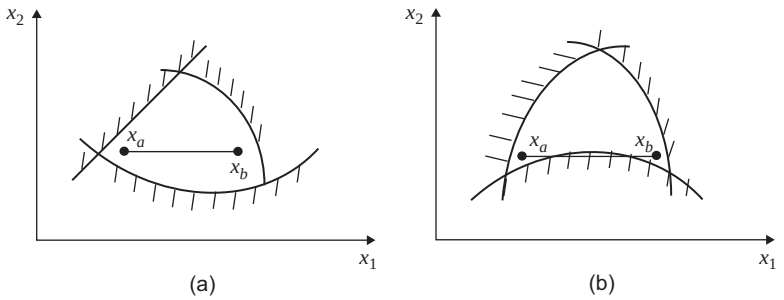


FIG. 12.9 Convexity for a two-variable problem. (a) Convex feasible region. (b) Nonconvex feasible region

12.8.1 Convexity

Constraint boundaries can also be plotted in the (x_1, x_2) parameter space, as illustrated in Fig. 12.9. If the constraints are not linear, there is a possibility that the feasible region may not be convex. A convex feasible region, illustrated in Fig. 12.9(a), is one in which any point on a straight line between any two points inside the feasible region also lies within the feasible region. This can be stated mathematically as:

$$x = \alpha x_a + (1 - \alpha)x_b \in \text{FR}$$
$$\forall\, x_a,\, x_b \in \text{FR},\ 0 < \alpha < 1 \tag{12.7}$$

where

x_a, x_b = any two points belonging to the feasible region
FR = the set of points inside the feasible region bounded by the constraints
α = a constant

If any two points in the feasible region can be found such that some point on a straight line between them lies outside of the feasible region, then the feasible region is nonconvex, as illustrated in Fig. 12.9(b).

The importance of convexity is that problems with a convex feasible region are more easily solved to a global optimum. Problems with nonconvex feasible regions are prone to convergence to local minima. Nonconvexity is common in chemical engineering problems due to the nonlinear nature of many of the equality constraint equations.

12.8.2 Searching in two dimensions

The procedures for searching in two dimensions are mostly extensions of the methods used for single-variable line searches:

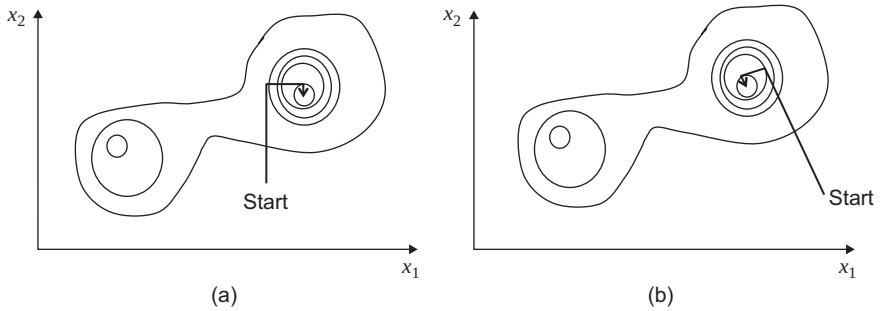


FIG. 12.10 Search methods. (a) Univariate search. (b) Steepest descent.

1. Find an initial solution (x_1, x_2) inside the feasible region.
2. Determine a search direction.
3. Determine step lengths δx_1 and δx_2.
4. Evaluate $z = f(x_1 + \delta x_1, x_2 + \delta x_2)$.
5. Repeat steps 2 to 4 until convergence.

If x_1 and x_2 are varied one at a time, then the method is known as a univariate search and is the same as carrying out successive line searches in each parameter. If the step length is determined so as to find the minimum with respect to the variable searched, then the calculation steps towards the optimum, as shown in Fig. 12.10(a). This method is simple to implement, but can be very slow to converge. Other direct methods include pattern searches, such as the factorial designs used in statistical design of experiments (see, for example, Montgomery, 2012), the EVOP method (Box, 1957), and the sequential simplex method (Spendley et al., 1962).

Indirect methods can also be applied to problems with two or more decision variables. In the steepest descent method (also known as the gradient method), the search direction is along the gradient at point (x_1, x_2), that is, orthogonal to the contours of $f(x_1, x_2)$. A line search is then carried out to establish a new minimum point where the gradient is reevaluated. This procedure is repeated until the convergence criterion is met, as shown in Fig. 12.10(b).

12.8.3 Problems in multivariable optimization

Some common problems that are encountered in multivariable optimization can be described for a two-variable problem and are illustrated in Fig. 12.11. In Fig. 12.11(a), the shape of the contours is such that a univariate search would be very slow to converge. Using an indirect method such as steepest descent would be more appropriate in this case. Fig. 12.11(b) shows the problem of convergence to a local optimum. In this scenario, different answers are obtained for different initial solutions. This problem can be overcome by using pattern searches with a larger grid or by using probabilistic methods such as simulated annealing or genetic algorithms that introduce some possibility of moving away from a local optimum. An introduction to probabilistic methods is given in Diwekar (2008). Probabilistic methods are also useful when faced with a nonconvex feasible region, as pictured in Fig. 12.11(c).

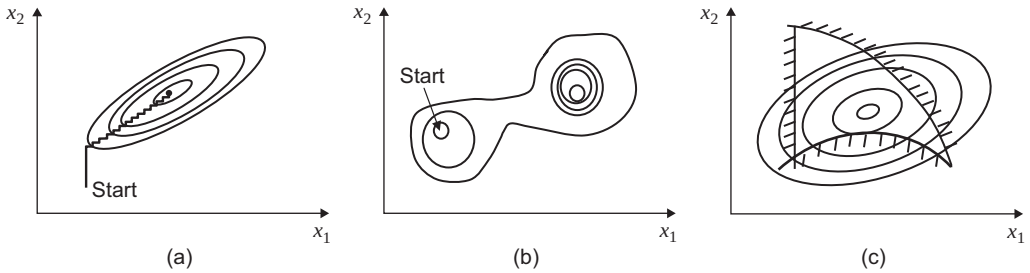


FIG. 12.11 Common problems in multivariable optimization. (a) Slow convergence. (b) Convergence to local optimum. (c) Nonconvex feasible region.

12.8.4 Multivariable optimization

When there are more than two decision variables, it is much harder to visualize the parameter space, but the same issues of initialization, convergence, convexity, and local optima are faced. The solution of large multivariable optimization problems is at the core of the field of operations research. Operations research methods are widely used in industry, particularly in manufacturing facilities, as discussed in Section 12.12.

The following sections give only a cursory overview of this fascinating subject. Readers who are interested in learning more should refer to Hillier and Lieberman (2014) and the other references cited in this chapter.

12.9 Linear programming

A set of continuous linear constraints always defines a convex feasible region. If the objective function is also linear and $x_i > 0$ for all x_i, then the problem can be written as a linear program (LP). A simple two-variable illustration of an LP is given in Fig. 12.12.

Linear programs always solve to a global optimum. The optimum must lie on the boundary at an intersection between constraints, which is known as a *vertex* of the feasible region. The inequality constraints that intersect at the optimum are said to be active and have $h(\mathbf{x}) = 0$, where $\mathbf{x}$ is the vector of decision variables.

Many algorithms have been developed to solve LPs, of which the most widely used are based on the SIMPLEX algorithm developed by Dantzig (1963). The SIMPLEX method introduces slack and surplus variables to transform the inequality constraints into equalities. For example, if:

$$x_1 + x_2 - 30 \leq 0$$

we can introduce a slack variable, S_1, and write:

$$x_1 + x_2 - 30 + S_1 = 0$$

The resulting set of equalities is solved to obtain a feasible solution, in which some of the slack and surplus variables will be zero, corresponding to active constraints. The algorithm then searches the vertices of the feasible region, decreasing the objective at each step until the optimum is reached. Details of the SIMPLEX method are given in most optimization or operations research textbooks. See, for example, Hillier and Lieberman (2014) or Edgar and Himmelblau (2001). There have been many improvements to the SIMPLEX algorithm over the years, but it is still the method used in most commercial solvers.

Some problems that can occur in solving LPs are illustrated in Fig. 12.13. In Fig. 12.13(a), the contours of the objective function are exactly parallel to one of the constraints. The problem is said to be degenerate and has an infinite number of solutions along the line of that constraint. Fig. 12.13(b) shows a problem where the feasible region is unbounded. This situation does not usually occur in engineering design unless the problem has been badly formulated. The situation in Fig. 12.13(c) is more common, in which the problem is overconstrained and there is no feasible region.

Linear programming can be used to solve very large problems, with thousands of variables and constraints. The method is widely used in operations, particularly in optimization of oil refineries and petrochemical plants. It is used a lot less in design, as design problems almost inevitably contain many nonlinear equations.

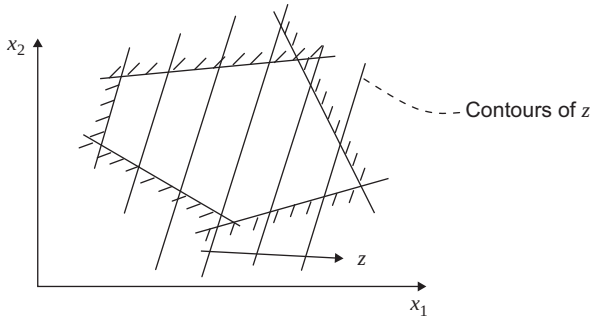


FIG. 12.12 A linear program.

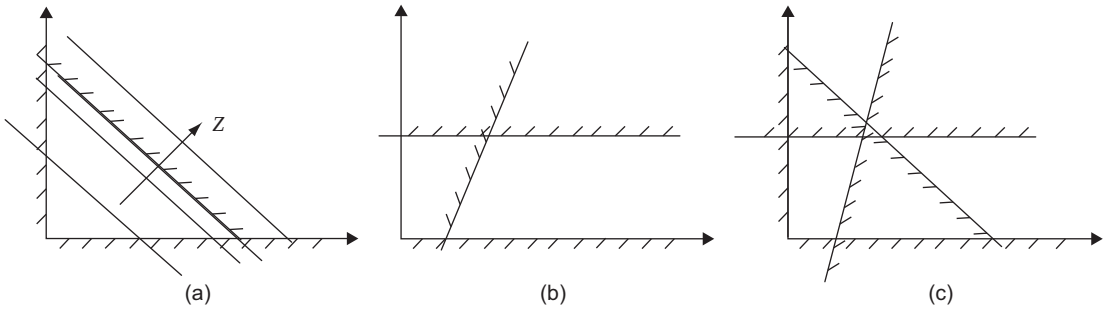


FIG. 12.13 Problems in linear programming. (a) Objective function parallel to a constraint (degenerate problem). (b) Feasible region unbounded. (c) No feasible region.

12.10 Nonlinear programming

When the objective function and/or the constraints are nonlinear, the optimization must be solved as a nonlinear program (NLP). Three main methods are used for solving an NLP.

12.10.1 Successive linear programming

In successive linear programming (SLP), $f(x)$, $\mathbf{g}(\mathbf{x})$, and $\mathbf{h}(\mathbf{x})$ are linearized at an initial point. The resulting LP is solved to give an initial solution, and $f(x)$, $\mathbf{g}(\mathbf{x})$, and $\mathbf{h}(\mathbf{x})$ are linearized again at the new point. The procedure is then repeated until convergence. If the new point is outside the feasible region, the nearest point lying inside the feasible region is used.

With SLP there is no guarantee of convergence or global optimality. The method is widely used, nonetheless, as it is a simple extension of linear programming. It should be noted that whenever discontinuous linear functions are used to approximate a nonlinear function, the problem behaves like an SLP. There is no guarantee of convexity or convergence to the optimal solution.

12.10.2 Successive quadratic programming

The successive quadratic programming (SQP) algorithm is similar to SLP, but instead approximates $f(x)$ as a quadratic function and uses quadratic programming methods that give faster convergence than SLP. SQP works well for highly NLPs with relatively few variables, for example, optimizing a process simulation or the design of a single piece of equipment. Biegler et al. (1997) suggest SQP is the best method for problems with fewer than 50 variables and where the gradients must be found numerically.

12.10.3 Reduced gradient method

Reduced gradient methods are related to the SIMPLEX algorithm. The method linearizes the constraints and introduces slack and surplus variables to transform the inequalities into equalities. The n-dimensional vector $\mathbf{x}$ is then partitioned into $n - m$ independent variables, where m is the number of constraints. A search direction is determined in the space of the independent variables, and a quasi-Newton method is used to determine an improved solution of $f(x)$ that still satisfies the nonlinear constraints. If all the equations are linear, this reduces to the SIMPLEX method (Wolfe, 1962). Various algorithms have been proposed, using different methods for carrying out the search and returning to a feasible solution, for example, the generalized reduced gradient (GRG) algorithm (Abadie & Guigou, 1969) and the MINOS algorithm (Murtagh & Saunders, 1978, 1982).

Reduced gradient methods are particularly effective for sparse problems with a large number of variables. A problem is said to be sparse if each constraint involves only a few of the variables. This is a common situation in design problems, where many of the constraints are written in terms of only one or two variables. Reduced gradient methods also work better when many of the constraints are linear, as less computational time is spent linearizing constraints and returning the solution to the feasible region. Because of the decomposition of the problem, fewer calculations are required per iteration, particularly if analytical expressions for the gradients are known (which is usually not the case in design). The reduced gradient method is often used in optimizing large spreadsheet models that contain many linear constraints.

All of the nonlinear programming algorithms can suffer from the convergence and local optima problems described in Section 12.8.3. Probabilistic methods such as simulated annealing and genetic algorithms can be used if it is suspected that the feasible region is nonconvex or multiple local optima are present.

12.11 Mixed-integer programming

Many of the decisions faced in operations involve discrete variables. For example, if we calculate that we need to ship 3.25 trucks of product from plant A to plant B each week, we could send 3 trucks for 3 weeks and then 4 trucks in the fourth week, or we could send 4 trucks each week, with the fourth truck only one-quarter filled, but we cannot send 3.25 trucks every week. Some common operational problems involving discrete variables include:

- Production scheduling: Determine the production schedule and inventory to minimize the cost of meeting demand. This is particularly important for batch plants, when the plant can make different products.
- Transshipment problems and supply chain management: Satisfy demands at different producing plants and sales destinations from different supply points, warehouses, and production facilities. Shipping quantities are often constrained to certain size lots corresponding to rail tankers, road tankers, drums, etc.
- Assignment problems: Schedule workers to different tasks.

Discrete variables are also sometimes used in process design, for example, the number of trays or the feed tray of a distillation column, and in process synthesis, to allow selection between flowsheet options, as described later.

Discrete decisions are addressed in operations research by introducing integer variables. When integer variables are introduced, an LP becomes a mixed-integer linear program (MILP) and a nonlinear program becomes a mixed-integer nonlinear program (MINLP). Binary integer variables are particularly useful, as they can be used to formulate rules that enable the optimization program to choose between options. For example, if we define y as a binary integer variable such that:

if $y = 1$ a feature exists in the optimal solution, and
if $y = 0$ the feature does not exist in the optimal solution,

then we can formulate constraint equations such as:

$\sum_{i=1}^{n} y_i = 1$ choose only one of n options
$\sum_{i=1}^{n} y_i \leq m$ choose at most m of n options
$\sum_{i=1}^{n} y_i \geq m$ choose at least m of n options
$y_k - y_j \leq 0$ if item k is selected, item j must be selected, but not vice versa

$$\left.\begin{array}{l} g_1(x) - M y \leq 0 \\ g_2(x) - M(1-y) \leq 0 \\ M \text{ is a large scalar value} \end{array}\right\} \quad \text{either } g_1(x) \leq 0 \text{ or } g_2(x) \leq 0$$

The last rule listed can be used to select between alternative constraints.

12.11.1 Mixed-integer programming algorithms

Although integer variables are convenient for problem formulation, if too many integer variables are used, the number of options explodes in a combinatorial manner and solution becomes difficult. Mixed-integer problems can be solved efficiently using methods such as the "branch and bound" algorithm. The branch and bound method starts by treating all integer variables as continuous and solving the resulting LP or NLP to give a first approximation. All integer variables are then rounded to the nearest integer to give a second approximation. The problem is then partitioned into two new integer problems for each integer variable that had a nonintegral solution in the first

approximation. In one branch a constraint is added that forces the integer variable to be greater than or equal to the next highest integer, whereas in the other branch a constraint is added that forces the variable to be equal to or less than the next lowest integer. For example, if a variable was found to have an optimal value $y = 4.4$ in the first approximation, then the new constraints would be $y \geq 5$ in one branch and $y \leq 4$ in the other. The branched problems are then solved to give new first approximations, and the branching procedure is repeated until an integer solution is found.

When an integer solution is found, it is used to set a bound on the value of the objective. For example, in a minimization problem, the optimal solution must be less than or equal to the bound set by this integral solution. Consequently, all branches with greater values of the objective can be discarded, as forcing the variables in these branches to integer values will lead to deterioration in the objective rather than improvement. The procedure then continues branching on all the nonintegral integer variables from each first approximation, setting new bounds each time an improved integer solution is found, until all of the branches have been bounded and the optimal solution has been obtained. See Hillier and Lieberman (2014) or Edgar and Himmelblau (2001) for details of the algorithm and examples of its application.

The branch and bound method can be used for MINLP problems, but it requires solving a large number of NLP problems and is therefore computationally intensive. Instead, methods such as the Generalized Benders' Decomposition and Outer Approximation algorithms are usually preferred. These methods solve a master MILP problem to initialize the discrete variables at each stage and then solve an NLP subproblem to optimize the continuous variables. Details of these methods are given in Floudas (1995), Biegler et al. (1997), and Diwekar (2008).

12.11.2 Superstructure optimization

Binary integer variables can be used to formulate optimization problems that choose between flowsheet options. For example, consider the problem of selecting a reactor. We can set up a unit cell consisting of a well-mixed reactor, a plug-flow reactor (PFR), and a bypass in parallel, each with a valve upstream, as illustrated in Fig. 12.14(a). If a binary variable is used to describe whether the valve is open or closed and a constraint is introduced such that only one of the valves is open, then the optimization will select the best option. A set of such unit cells can be built into a superstructure, incorporating additional features such as recycles, as shown schematically in Fig. 12.14(b). A more rigorous superstructure that encompasses other options such as side-stream feeds to the plug-flow reactor (PFR) was developed by Kokossis and Floudas (1990).

The optimization of such a superstructure can identify reactor networks or mixing arrangements that would not be intuitively obvious to the design engineer. Similar superstructure formulations have been proposed for other process synthesis problems such as distillation column sequencing, design of heat-exchange networks, and design of site utility systems. Biegler et al. (1997) give an excellent overview of the use of superstructure-based methods in process synthesis.

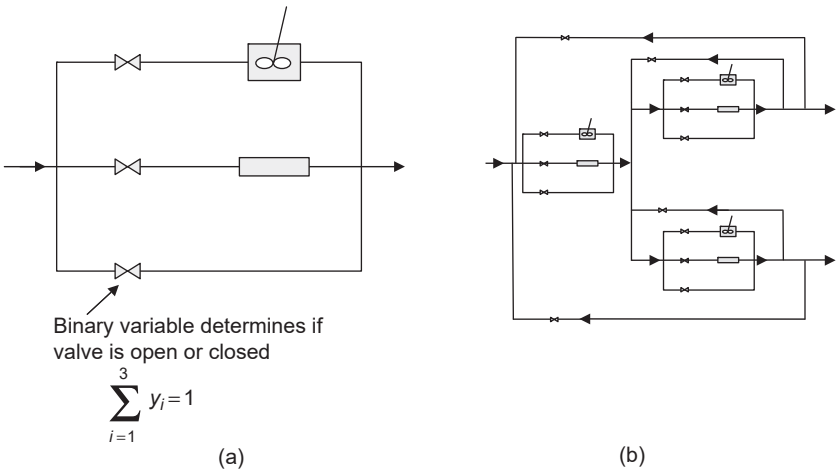


FIG. 12.14 Application of integer programming to reactor design. (a) Unit cell of reactor options. (b) Superstructure of unit cells and recycles.

12.12 Optimization in industrial practice

12.12.1 Optimization of process operations

Perhaps not surprisingly, operations research methods are widely used in process operations. Few manufacturing plants do not use LP or MILP tools for planning and scheduling. Supply chain management is very important to economic performance, and is usually carried out using large MILP models. The models used in industry for these purposes are often not very sophisticated, but proper formulation of constraints and the ability to solve robustly with a large number of variables are usually more important features of tools for these applications.

The use of operations research methods for plant and supply chain applications is taught as part of the industrial engineering curriculum in most universities. Chemical engineers considering a career in manufacturing would be well advised to develop a solid grounding in these methods.

12.12.2 Optimization of batch and semicontinuous processes

In batch operation, there will be periods when product is being produced, followed by nonproductive periods when the product is discharged and the equipment prepared for the next batch. The rate of production will be determined by the total batch time, productive plus nonproductive periods.

$$\text{Batches per year} = \frac{8760 \times \text{plant attainment}}{\text{batch cycle time}} \tag{12.8}$$

where the "plant attainment" is the fraction of the total hours in a year (8760) that the plant is in operation.

$$\begin{aligned} \text{Annual production} &= \text{quantity produced per batch} \times \text{batches per year.} \\ \text{Cost per unit of production} &= \frac{\text{annual cost of production}}{\text{annual production rate}} \end{aligned} \tag{12.9}$$

With many batch operations, the production rate decreases during the production period; for example, batch reactors and plate and frame filter presses. There is then an optimum batch size, or optimum cycle time, that gives the minimum cost per unit of production.

For some continuous processes, the period of continuous production will be limited by gradual changes in process conditions. Examples include the deactivation of catalysts or the fouling of heat-exchange surfaces. Production is lost during the periods when the plant is shut down for catalyst renewal or equipment cleaning. As with batch processes, there is an optimum cycle time to give the minimum production cost. The optimum time between shut-downs can be found by determining the relationship between cycle time and cost per unit of production (the objective function) and using one of the optimization techniques outlined in this section to find the minimum.

With discontinuous processes, the period between shut-downs will usually be a function of equipment size. Increasing the size of critical equipment will extend the production period, but at the expense of increased capital cost. The designer must strike a balance between the savings gained by reducing the nonproductive period and the increased investment required.

In some batch plants several trains of identical equipment are operated in a sequence that allows some degree of heat recovery or enables downstream equipment to operate continuously. In this type of plant the time allowed for each operation in the sequence is optimized so that an overall schedule for the plant can be developed. Scheduling of batch processes is described in Biegler et al. (1997).

12.12.3 Optimization in process design

Few, if any, industrial designs are rigorously optimized. This is because:

1. The cost of building rigorous models of reactor kinetics and hydraulics that give accurate prediction of by-product yields is usually not justified. The amount of time available for the project is usually insufficient for such models to be built. The errors introduced by uncertainty in the process models may be much larger than the differences in performance predicted for different designs.
2. The uncertainty in the forecasts of future prices is usually so large that it dominates most differences between design alternatives.

3. Regardless of the quality of the tools used or the experience of the estimator, it is usually impossible to make a capital cost estimate within ±15% without completing a substantial amount of design work (see Chapter 7). Many design decisions are thus made on the basis of sketchy cost estimates. The cost of going back and revisiting these design decisions at a later stage in the project when more design detail is available is usually not justified.
4. Criteria such as safety, operability, reliability, and flexibility are of vital importance in process design. These features make the design more robust to variations in the design assumptions and operating requirements. A safe, operable, and reliable plant will often require more expense above the cost of the economically "optimal" design. This extra expense is difficult to trade off against the nonfinancial benefits of having a process that is easier to run.
5. In most cases there are several "near-optimal" designs. The difference between the values of the objective obtained for each of these is often not statistically significant, given the errors in prices, cost estimates, and yields.

In industrial process design, optimization usually involves carrying out sufficient analysis to be confident that the design is reasonably close to the optimum. The most important things for the design engineer to understand are:

1. What are the constraints on the design?
2. Which constraints are hard (inviolable) and which are soft (can be modified)?
3. Where are the discontinuities in cost? For example, what conditions cause a change to a more costly metallurgy or a different design code?
4. What are the main design trade-offs?
5. How does the objective function vary with the main process parameters?
6. What are the major cost components of the process (both capital and operating costs), and what radical changes could be made to the process to reduce these costs?

Experienced design engineers usually think through these questions carefully to satisfy themselves that their design is "good enough." Only very occasionally do they formulate an optimization problem and solve it rigorously.

Example 12.1

Optimize the design of a distillation column to separate 225 metric tons per hour of an equimolar mixture of benzene, toluene, ethylbenzene, paraxylene, and orthoxylene with minimum total annualized cost. The feed is a saturated liquid at 330 kPa. The recovery of toluene in the distillate should be greater than 99%, and the recovery of ethylbenzene in the bottoms should be greater than 99%.

Solution

The first step is to determine the design factor. If we assume a design factor of 10%, then the equipment should be designed for a flow rate of 248 metric tons per hour (te/h). This flow rate is used in simulating the process for the purpose of sizing equipment, but energy consumption must be based on the reboiler and condenser duties expected for a 225 te/h feed rate.

This is a single distillation column, which is easy to model in any of the commercial simulation programs. UniSim (Honeywell, Inc.) was used for the purpose of this example. The simulation was set up using the component recoveries of toluene and ethylbenzene as column specifications, which gave rapid convergence. Tray sizing calculations were run using the UniSim tray sizing utility. A tray spacing of 0.61 m (2 ft) was assumed, and other tray parameters were left at the UniSim default values. Two meters were added to the column height to allow space for a sump and demister. Sieve trays were used, and the stage efficiency was assumed to be 80%. Details of the column simulation and design are given in Examples 4.6 and 4.7.

To optimize the design, we need to formulate an objective function. The distillation column has the following cost components:

- Capital costs: column shell, internals, condenser, receiver drum, reboiler, pumps, piping, instrumentation, structure, foundations, etc.
- Operating costs: cost of heating for the reboiler and cost of cooling for the condenser

The purchased equipment costs can be estimated based on information from the process simulation using the cost correlations given in Chapter 7. The column shell is a pressure vessel, and the design can be completed using the methods given in Chapter 14. The details of how to complete these calculations are not important here, but Example 14.2 and Example 7.3 provide detailed explanations of the method followed. Carbon steel construction was assumed. The purchased equipment costs can be converted into an installed capital cost by multiplying by an installation factor. For the purposes of this example, the installation factor can be assumed to be 4.0; see Section 7.6. The installed capital costs can be converted into an annual capital charge by dividing by 3, using a rule of thumb that is developed in Section 9.7.

TABLE 12.2 Optimization results

Iteration number	1	2	3	4	5	6	7	8	9
Number of trays	40	90	120	70	80	76	84	80	80
Feed tray	20	45	60	35	40	38	42	27	53
Column height (m)	26.4	56.9	75.2	44.7	50.8	48.4	53.2	50.8	50.8
Column diameter (m)	5.49	4.42	4.42	4.42	4.42	4.42	4.42	4.42	4.57
Reflux ratio	3.34	2.50	2.48	2.57	2.52	2.54	2.51	2.48	2.78
Reboiler duty, Q_r (MW)	34.9	28.3	28.2	28.8	28.5	28.6	28.4	28.2	30.4
Condenser duty, Q_c (MW)	33.9	27.3	27.2	27.8	27.5	27.6	27.4	27.2	29.4
Annualized capital cost (MM$/y)	0.82	0.95	1.25	0.83	0.89	0.87	0.91	0.89	0.94
Annual energy cost (MM$/y)	8.59	6.96	6.93	7.10	7.01	7.04	6.99	6.93	7.50
Total annualized cost (MM$/y)	9.41	7.91	8.18	7.93	7.900	7.905	7.904	7.82	8.44

The operating costs are simple to estimate from the condenser and reboiler duties if the cost of energy is known. For this example, the cost of heat is taken as \$7.5/GJ and the cost of cooling is \$0.2/GJ.

The objective function can then be written as:

$$\text{Min.: Total annualized cost (TAC)} = \text{cost of heating} + \text{cost of cooling} + \text{annualized capital cost}$$

$$= 5.5Qr + 0.2Qc + (4/3)\,(\Sigma\ \text{purchased equipment costs})$$

where:

Q_r = annual reboiler energy consumption (GJ/yr)
Q_c = annual condenser energy consumption (GJ/yr)

The optimization problem is strictly a MINLP, as we need to consider discrete variables (number of trays, feed tray) as well as continuous variables (reflux ratio, reboiler duty, etc.). This problem is actually relatively easy to formulate and solve rigorously, but instead we will step through the calculation to illustrate how an experienced industrial designer would approach the problem.

Table 12.2 gives the results of several iterations of the optimization.

1. To begin, we need to find a feasible solution. As an initial guess we can use 40 trays with the feed on tray 20. The column converges with a reflux ratio of 3.34 and diameter 5.49 m. This is large, but not unreasonable for such a high flow rate. Looking at the components of the total annualized cost, the capital is contributing \$0.8 MM/yr and energy is contributing \$8.6 MM/yr, so the costs are dominated by energy cost. It is clear that adding more stages and reducing the reflux ratio will reduce the total cost. (If capital costs were dominating, then we would reduce the number of stages.) There is no upper hard constraint on column height, but there is a soft constraint. At the time of writing there are only 14 cranes in the world that can lift a column taller than 80 m. There are 48 cranes that can lift a column up to 60 m. We can therefore expect that the cost of lifting a column >60 m height will go up as it becomes more expensive to rent the necessary equipment for installation. We can start by assuming a soft constraint that the maximum height must be less than 60 m.
2. Using 90 trays with feed on tray 45 gives a reflux ratio of 2.5 and diameter 4.42 m. The column height is 56 m, which allows some space for vessel supports and clearance for piping at the column base and still comes in under the 60-m target. The capital cost increases to \$0.95 MM/yr, while energy cost is reduced to \$6.96 MM/yr, giving a total annualized cost of \$7.91 MM/yr and savings of \$1.5 MM/yr relative to the initial design.
3. We should explore whether going to an even taller column would make sense. We can investigate this by increasing the installation factor from 4 to 5 for the column shell to allow for the higher cost of using one of the larger cranes. If we increase the number of trays to 120, the column height is 75 m, which will give a total height of close to 80 m when installed. The total annualized cost increases to \$8.2 MM/yr, so we can conclude that it is probably not economical to go to a total height above 60 m. We can notice, though, that the reflux ratio didn't change much

when we added extra trays. This suggests that we are getting close to minimum reflux. It might therefore be worth backing off from the maximum column height constraint to see if there is an optimum number of trays.

4. Adding a design with 70 trays and feed on tray 35 (roughly halfway between 40 and 90) gives reflux ratio 2.57 and total annualized cost \$7.94 MM/yr. This is not an improvement on the 90-tray design, so the optimum must be between 70 and 90 trays.
5. A design with 80 trays and feed on tray 40 (halfway between 70 and 90) gives reflux ratio 2.52 and total annualized cost \$7.900 MM/yr. This is better than 70 or 90 trays. If we wanted to proceed further to establish the optimum, we could continue reducing the search space using a regular search until we get to the optimum number of trays. Instead, an experienced designer would note that the difference in cost within the range examined (\$0.03 MM/yr) is relatively small compared with the error in the capital cost estimate ($\pm$30%, or \$0.29 MM/yr). Because the optimum appears to be fairly flat with respect to the number of trays over the range 70 to 90, it is reasonable to take the optimum as 80 trays. (As a confirmation, iterations 6 and 7, with 76 and 84 trays, indicate that the optimum indeed lies at 80 $\pm$ 2 trays).
6. Having fixed the number of trays at 80, we should now optimize the feed tray. We start by adding two new points, with the feed tray at trays 27 and 53. These give total annualized costs of \$7.82 MM/yr and \$8.43 MM/yr, respectively. The minimum cost is given by the lower bound on feed tray location. If we try a higher feed tray (say, tray 26) the UniSim tray sizing utility gives a warning "head loss under downcomers is too large." We could overcome this warning by modifying the tray design, but once again we can notice that the annualized cost savings that we have gained by optimizing feed tray (\$0.08 MM/yr) is small compared with the error in the capital cost, so the design with feed tray 27 is close enough to optimum.

The column design is thus set at 80 trays, with feed on tray 27, giving a column 50.8 m high and 4.42 m diameter.

The solution obtained is "good enough" but is not rigorously optimal. Several possible variations in flow scheme were not considered. For example, we could have examined use of feed pre-heat, intermediate-stage condensers or reboilers, or more efficient column internals such as high-efficiency trays or structured packing. The column cost may also be reduced if different diameters or different internals were used in the rectifying and stripping sections. In the broader context of the process, it may be possible to supply the heat required for the reboiler using heat recovered from elsewhere in the process, in which case the cost of energy will be reduced and the capital energy trade-off will be altered. In the overall process context, we could also question whether the column needs such high recoveries of toluene and ethylbenzene, because the high recoveries clearly lead to a high reflux rate and column energy cost.

12.13 References

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12.14 Nomenclature

		Dimensions in $MLTθ
A	A constant	—
B	A constant	—
$f(x)$	General function of x	—
$f'(x)$	First derivative of function of x with respect to x	—
$f''(x)$	Second derivative of function of x with respect to x	—
FR	The set of points contained in a feasible region	—
g(x)	A mi vector of inequality constraints	—
$g(x)$	General inequality constraint equation in x	—
h(x)	A m_e vector of equality constraints	—
$h(x)$	General equality constraint equation in x	—
h	Step length in a search algorithm	—
M	A large scalar constant	—
m	Number of constraints	—
m_e	Number of equality constraints	—
m_i	Number of inequality constraints	—
n	Number of variables	—
Q_c	Condenser duty in distillation	$\mathbf{ML^2T^{-3}}$
Q_r	Reboiler duty in distillation	$\mathbf{ML^2T^{-3}}$
S_1, S_2 …	Slack and surplus variables	—
T	Temperature	θ
T_{alloy}	Maximum allowed temperature for an alloy	θ
T_A, T_B, T_C	Maximum allowed temperature for alloys A, B, and C	θ
U	Overall heat transfer coefficient	$\mathbf{MT^{-3}\theta^{-1}}$
X	A vector of n decision variables	—
x_1, x_2 …	Continuous variables	—
y_1, y_2 …	Integer (discrete) variables	—
z	The objective (in optimization)	—
α	A constant between 0.0 and 1.0	—
ϵ	Fraction of search range or tolerance for convergence	—
ΔT	Temperature difference	θ
$\Delta T_{optimum}$	The optimal minimum temperature approach in heat recovery	θ

		Dimensions in $MLT\theta$
δx_1, δx_2	Small increments in x_1 and x_2	—
ω	Ratio used in golden-section search (= 0.381966)	—
Suffixes		
D1	lower side of a discontinuity	—
D2	upper side of a discontinuity	—
i	i^{th} variable	—
j	j^{th} variable	—
k	k^{th} iteration	—
L	lower bound	—
S	stationary point	—
U	upper bound	—

12.15 Problems

12.1. A separator divides a process stream into three phases: a liquid organic stream, a liquid aqueous stream, and a gas stream. The feed stream contains three components, all of which are present to some extent in the separated steams. The composition and flow rate of the feed stream are known. All the streams will be at the same temperature and pressure. The phase equilibrium constants for the three components are available.

a. How many design variables must be specified to calculate the output stream compositions and flow rates?

b. How would you optimize these variables if the objective of the separator were to maximize recovery of condensable components into the organic liquid stream? What constraints might limit the attainable recovery?

12.2. A rectangular tank with a square base is constructed from 5-mm steel plates. If the capacity required is 8 cubic meters, determine the optimum dimensions if the tank has:

a. a closed top

b. an open top

12.3. Estimate the optimum thickness of insulation for the roof of a house given the following information. The insulation will be installed flat on the attic floor.

Overall heat transfer coefficient for the insulation as a function of thickness, *U* values (see Chapter 19):

thickness, mm	0	25	50	100	150	200	250
U, $Wm^{-2}K^{-1}$	20	0.9	0.7	0.3	0.25	0.20	0.15

The cost of insulation, including installation, is \$120/m^3. Capital charges (see Chapter 9) are 20% per year. The cost of fuel, allowing for the efficiency of the heating system, is \$8/GJ. The cost of cooling is \$5/GJ. Average temperatures for any region of the United States or Canada can be found online at www.weather.com (under the averages tab). Assume the house is heated or cooled to maintain an internal temperature in the range 70 to 80 °F.

Note: The rate at which heat is being lost or gained is given by $U \times \Delta T$, W/m^2, where *U* is the overall coefficient and ΔT the temperature difference; see Chapter 19.

12.4. What is the optimum practical shape for an above-ground dwelling to minimize the heat losses through the building fabric? When is (or was) this optimum shape used? Why is this optimum shape seldom used in richer societies?

12.5. Hydrogen is manufactured from methane by either steam reforming (reaction with steam) or partial oxidation (reaction with oxygen). Both processes are endothermic. What reactor temperature and pressure would you expect to be optimal for these processes? What constraints might apply?

12.6. Ethylene and propylene are valuable monomers. A key step in the recovery of these materials is fractionation of the olefin from the corresponding paraffin (ethane or propane). These fractionation steps require refrigeration of the overhead condenser and very large distillation columns with many stages. Raising the pressure at which the column operates improves the performance of the refrigeration system, but increases the number of stages needed. Formulate the objective function for optimizing the recovery of ethylene from an ethylene–ethane mixture. What are the key constraints? What will be the main trade-offs?

12.7. If you had to design a plant for pasteurizing milk, what constraints would you place on the design?

12.8. A catalytic process was designed to make 150,000 metric tons per year of product with a net profit of $0.25/lb of product. The catalyst for the process costs $10/lb, and it takes 2 months to shut down the process, empty the old catalyst, reload fresh catalyst, and restart the process. The feed and product recovery and purification sections can be pushed to make as much as 120% of design basis capacity. The reactor section is sized with sufficient catalyst to make 100% of design basis when operated with fresh catalyst at 500 °F. The reactor can only be operated at temperatures up to 620 °F for safety reasons. The reactor weight hourly space velocity (lb of product per hour per lb of catalyst) is given by the equation:

$$\text{WHSV} = 4.0 \times 10^{6} \exp\left(\frac{-8000}{T}\right)\exp\left(-8.0 \times 10^{-5} \times t \times T\right)$$

where

t = time on stream in months
T = temperature

Find the optimal temperature versus time profile for the reactor and determine how long the process should be operated before the catalyst is changed out. (Hint: The initial temperature does not have to be 500 °F).

12.9. The portfolio of investment projects shown here has been proposed for a company for next year:

Project	Net present value (MM$)	Cost (MM$)
A	100	61
B	60	28
C	70	33
D	65	30
E	50	25
F	50	17
G	45	25
H	40	12
I	40	16
J	30	10

a. Develop a spreadsheet optimization program to select the optimal portfolio of projects to maximize total portfolio net present value (NPV), given a total budget of $100 million. (This is a simple MILP.)
b. How would the portfolio and NPV change if the budget were increased to $110 million?
c. Because of corporate cost-cutting, the budget is reduced to $80 million. Which projects are now funded, and what is the new NPV?
d. Based on your answers to parts a to c, can you draw any conclusions on which projects are likely to be funded regardless of the financial situation?
e. Can you see any problems with this project selection strategy? If so, how would you recommend they should be addressed?

CHAPTER

13

Equipment selection, specification, and design

KEY LEARNING OBJECTIVES

- Where to find information on process equipment
- How to obtain equipment information from vendors

13.1 Introduction

Part I of this book covered process design: the synthesis of the complete process as an assembly of units, each carrying out a specific process operation. In Part II, the selection, specification, and design of the equipment required to carry out these process operations is considered in more detail.

In practice, plant design and process design cannot be separated. The selection and specification of one piece of equipment will often require the use of additional equipment and thus have implications on the process flow diagram. For example, if a continuous dryer is selected for drying a solid product, it may be necessary to add a heater to pre-heat the drying gas, a cyclone or filter to recover solid fines from the off-gas, a cooler and flash drum to cool the off-gas and recover solvent, a vent scrubber to prevent solvent emissions, etc. The design team must understand all the flowsheet implications of equipment selection and design to arrive at an accurate cost estimate and process optimization.

This chapter gives a short introduction to the selection and design of process equipment and provides a guide to the following chapters. Most process operations are carried out in closed pressure vessels, which are addressed in Chapter 14. Chapter 15 discusses the design of chemical and biochemical reactors. Separation processes are covered in Chapters 16 and 17. Chapter 18 addresses operations that involve solids handling. Chapter 19 describes the design of equipment for heat transfer and Chapter 20 covers the transport and storage of fluids.

Each chapter and section of Part II is intended to be a stand-alone guide to the design of a particular operation, but in some cases cross-references to sections of other chapters are given to avoid duplication. Throughout Part II the emphasis is on selection and sizing of equipment, and it is assumed that the reader is familiar with the fundamentals of kinetics, thermodynamics, and transport processes. Further details on the scientific principles and theory that underlie the design and operation of process equipment can be found in the numerous textbooks cited in each section and in general books on unit operations, such as Chhabra and Gurappa (2019) and McCabe et al. (2004).

Capital cost correlations for each type of equipment are not given in Part II, as the determination of capital costs for all types of equipment was discussed in Chapter 7. Similarly, materials selection was covered in Chapter 6. Although the role of safety in design was described in Chapter 10, some additional safety issues that are specific to certain unit operations are covered in the relevant sections of Part II.

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13.2 Sources of equipment design information

13.2.1 Proprietary and nonproprietary equipment

The equipment used in the chemical process industries can be divided into two classes: proprietary and nonproprietary. Proprietary equipment, such as pumps, compressors, filters, centrifuges, and dryers, is designed and sold as standard catalogue items by specialist manufacturers. Nonproprietary equipment is designed as special, one-off, items for particular processes; for example, reactors, distillation columns and heat exchangers, and is custom-built by specialist fabricators.

Unless employed by one of the specialist equipment manufacturers, the chemical engineer is not normally involved in the detailed design of proprietary equipment. The chemical engineer's job will be to specify the process duty (flow rate, heat load, temperature, pressure, etc.) and then select an appropriate piece of equipment to meet that duty, consulting with the vendors to ensure that the equipment supplied is suitable. Proprietary equipment is often only made in certain standard sizes, and the design engineer must determine which size is best suited for the application or whether to use multiple units in parallel to accommodate the desired flow. Chemical engineers may be involved with the vendor's designers in modifying standard equipment for particular applications, for example, a standard tunnel dryer designed to handle particulate solids may be adapted to dry synthetic fibers. As was pointed out in Chapter 1, the use of standard off-the-shelf equipment, whenever possible, will reduce costs.

Reactors, columns, flash drums, decanters, and other vessels are usually designed as special items for a given project. In particular, reactor designs are usually unique, except where more or less standard equipment is used, such as an agitated, jacketed vessel. Distillation columns, vessels, and tubular heat exchangers, though nonproprietary items, will be designed to conform to recognized standards and codes; this reduces the amount of design work involved.

The chemical engineer's part in the design of "nonproprietary" equipment is usually limited to selecting and "sizing" the equipment. For example, in the design of a distillation column, the design engineer will typically determine the number of plates; the type and design of plate; diameter of the column; and the position of the inlet, outlet, and instrument nozzles. This information would then be transmitted, in the form of sketches and specification sheets, to the specialist mechanical design group, or the fabricator's design team, for detailed design.

It must be emphasized that companies that are engaged in the manufacture of chemicals, fuels, polymers, foods, and pharmaceuticals almost never build their own process equipment. The design engineers from the operating company usually provide specifications to detailed design groups at an engineering, procurement, and construction (EPC) company, who then subcontract the equipment manufacture to specialist equipment fabricators. Even one-of-a-kind items such as reactors, distillation columns, and heat exchangers are built by specialist manufacturers. The accurate transmission of design details is therefore very important, and the process industries have developed many standard specifications to facilitate information exchange with vendors. Standard specifications should be used whenever possible, as these lead to cheaper designs and reduce the risk of needing rework during construction.

13.2.2 Published information on process equipment

Technical literature

Descriptions and illustrations of most types of process equipment can be found in various handbooks: Green and Southard (2018), Schweitzer (1997), and Crouper et al. (2012). *Perry's Chemical Engineers' Handbook* remains the most comprehensive compilation of chemical engineering information. The online version provided by Knovel is the most accessible format. Many specialized books have been written on individual unit operations; these are cited throughout the following chapters.

Equipment manufacturers often write articles in the trade journals. Although these are primarily promotional, they can be quite informative. The trade journals also contain advertisements that can help identify manufacturers. Articles by equipment vendors are common in *Chemical Engineering* and *The Chemical Engineer* and appear somewhat less frequently in *Chemical Engineering Progress* and *Hydrocarbon Processing*. The journals usually contain a reader response card that can be faxed or mailed in to receive advertisers' brochures and sales literature. These can be used to build up a library of vendors' catalogues.

Every year the journal *Chemical Engineering* publishes a buyers' guide. The *Chemical Engineering Buyers' Guide* lists over 500 manufacturers and provides indexes by product type, company name, and trade name, as well as listing websites and contact information for industry associations. It can be used as a "yellow pages" of chemical industry suppliers, but like other directories, it is not fully comprehensive, as not all manufacturers will pay to be listed.

In the United Kingdom, a commercial organization, Technical Indexes Ltd., publishes the Process Engineering Index, which contains information from over 3000 manufacturers and suppliers of process equipment globally.

Online information

All equipment vendors now maintain an online presence, but there is a wide variation in the quality of the websites and the amount of information provided.

Several directory sites have been set up to serve the chemical and process industries. Of these, the best at time of writing is www.chemindustry.com, which has links to many vendors. More limited information is also available at www.chemengg.com and www.cheresources.com. A good site for finding new and used equipment for sale is www.equipnet.com.

Manufacturer's websites are usually easily located using online search engines and often provide details of equipment construction, standard sizes, available metallurgies, specification sheets, and performance information. The *Chemical Engineering Buyers' Guide* can also be used to identify vendor websites for specific equipment types. Manufacturers' association websites usually provide the most comprehensive listings of vendors; see, for example, the websites of the Valve Manufacturers' Association (www.vma.org), Tubular Exchanger Manufacturers' Association (http://tema.org), and Conveyor Equipment Manufacturers' Association (http://cemanet.org). Other manufacturers' associations are usually easy to find by searching the Internet.

Some equipment types are relatively easy to find using search engines ("crystallizer," "rotary agglomerator," "bioreactor," etc.), but locating the vendors of industrial plant can be more difficult when the equipment name is in common usage ("furnace," "dryer," "filter," "pump," etc.). In such cases, the best approach is to begin at one of the chemical engineering directory sites listed earlier.

13.3 Guide to equipment selection and design

Table 13.1 is a guide to the design of the most common types of process equipment. The numbers refer to the section of this book that provides design guidelines. Table 13.2 is a similar guide for separation processes, which have been grouped based on the phases that are separated. Capital cost correlations for most of the equipment listed in these tables can be found in Table 7.2.

TABLE 13.1 Guide to equipment design

Equipment type	Basic sizing	Detailed design
Reactors		
Basic reactors	15.2, 15.5	As pressure vessels,
Bioreactors	15.9	Chapter 14
Catalytic reactors	15.8	
Multiphase reactors	15.7	
Nonisothermal reactors	15.6	
Separation columns		
Absorption	16.2.4, 17.14	Shells as pressure vessels:
Distillation	17.2–17.13	Chapter 14
Extraction	17.16	Internals:
Single-stage flash	16.3, 17.3.3	Trays 17.12–17.13
Stripping	16.2.4, 17.14	Packing 17.14
Other separation processes		See Table 13.2
Heat exchange equipment		
Air coolers		19.16
Boilers, reboilers, vaporizers		19.11
Condensers		19.10
Fired heaters		19.17
Plate heat exchangers		19.12
Shell and tube exchangers		19.1–19.9
Transport equipment		
Compression of gases		20.6
Conveying of solids		18.3
Pumping of liquids		20.7
Solids handling equipment		
Size reduction (grinding)		18.9
Size enlargement (forming)		18.8
Heating and cooling solids		18.10

Numbers refer to the sections in this book.

TABLE 13.2 Separation processes

Major component		Minor Component: Solid		Minor Component: Liquid		Minor Component: Gas/Vapor	
Solid		Sorting	18.4	Pressing	18.6.5		
		Screening	18.4.1	Drying	18.7		
		Hydrocyclones	18.4.2				
		Classifiers	18.4.3				
		Jigs	18.4.4				
		Tables	18.4.5				
		Centrifuges	18.4.6				
		Dense media	18.4.7				
		Flotation	18.4.8				
		Magnetic	18.4.9				
		Electrostatic	18.4.10				
Liquid		Thickeners	18.6.1	Decanters	16.4.1	Stripping	16.2.4
		Clarifiers	18.6.1	Coalescers	16.4.3		17.14
		Hydrocyclones	18.6.4	Solvent extraction	16.5.6		
		Filtration	18.6.2	Leaching	16.5.6		
		Centrifuges	18.6.3	Chromatography	16.5.7		
		Crystallizers	16.5.2	Distillation	Chapter 17		
		Evaporators	16.5.1				
		Precipitation	16.5.3				
		Membranes	16.5.4				
		Reverse osmosis	16.5.4				
		Ion exchange	16.5.5				
		Adsorption	16.5.7				
Gas/Vapor		Gravity Settlers	18.5.1	Separating vessels	16.3	Adsorption	16.2.1
		Impingement Settlers	18.5.2	Demisting pads	16.3	Absorption	16.2.4
				Cyclones	18.5.3		17.14
		Cyclones	18.5.3	Wet scrubbers	18.5.5	Membranes	16.2.2
		Filters	18.5.4	Electrostatic precipitators	18.5.6	Cryogenic distillation	16.2.3
		Wet scrubbers	18.5.5				Chapter 17
		Electrostatic precipitators	18.5.6			Condensation	16.2.5

Numbers refer to the sections in this book. The terms major and minor component only apply where different phases are to be separated (i.e., not to those on the diagonal). Note that separation processes include processes for separating phases, as well as for recovering one or more components from a mixture.

13.4 References

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CHAPTER

14

Design of pressure vessels

KEY LEARNING OBJECTIVES

- What factors a process engineer must consider when setting specifications for a pressure vessel
- How pressure vessels are designed and built and what determines the vessel wall thickness
- How to design and size vessels for use as reactors, columns, separators, and other process uses
- How codes and standards are used in pressure vessel design

14.1 Introduction

This chapter covers those aspects of the mechanical design of chemical plants that are of particular interest to chemical engineers. The main topic considered is the design of pressure vessels. The design of storage tanks is also discussed briefly. Most reactors, separation columns, flash drums, heat exchangers, surge tanks, and other vessels in a chemical plant will need to be designed as pressure vessels, so this topic is relevant to a broad range of process equipment.

The chemical engineer will not usually be called on to undertake the detailed mechanical design of a pressure vessel. Vessel design is a specialized subject and will be carried out by mechanical engineers who are conversant with the current design codes and methods of stress analysis. However, the chemical engineer will be responsible for developing and specifying the basic design information for a particular vessel and needs to have a general appreciation of pressure vessel design to work effectively with the specialist designer.

Another reason why the process engineer must have an appreciation of methods of fabrication, design codes, and other constraints on pressure vessel design is because these constraints often dictate limits on the process conditions. Mechanical constraints can cause significant cost thresholds in design, for example, when a costlier grade of alloy is required above a certain temperature.

The basic data needed by the specialist designer will be:

1. Vessel function
2. Process materials and services
3. Operating and design temperature and pressure
4. Materials of construction
5. Vessel dimensions and orientation
6. Type of vessel heads to be used

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7. Openings and connections required
8. Specification of heating and cooling jackets or coils
9. Type of agitator
10. Specification of internal fittings

An elementary understanding of pressure vessel design is needed in the preliminary stages of design, as most correlations for pressure vessel costs are based on the weight of metal required and hence require an estimate of the vessel wall thickness, as well as its volume. In many cases, the required wall thickness will be determined by the combination of loads acting on the vessel rather than internal pressure alone.

A data sheet for pressure vessel design is given in Appendix G, available online at www.elsevier.com/books-and-journals/book-companion/9780128211793. Pressure vessel information is also included in the data sheets for fixed-bed reactors, vapor–liquid contactors, and heat exchangers.

There is no strict definition of what constitutes a pressure vessel, and different codes and regulations apply in different countries; however, it is generally accepted that any closed vessel over 150 mm diameter subject to a pressure difference of more than 0.5 bar should be designed as a pressure vessel.

It is not possible to give a completely comprehensive account of vessel design in one chapter. The design methods and data given should be sufficient for the preliminary design of conventional vessels, for the chemical engineer to check the feasibility of a proposed equipment design, to estimate the vessel cost for an economic analysis, and to determine the vessel's general proportions and weight for plant layout purposes. For a more detailed account of pressure vessel design, the reader should refer to the books by Singh and Soler (1992), Escoe (1994) and Moss and Basic (2013). Other useful books on the mechanical design of process equipment are listed in the bibliography at the end of this chapter.

An elementary understanding of the principles of the "strength of materials" (mechanics of solids) will be needed to follow this chapter. Readers who are not familiar with the subject should consult one of the many textbooks available, such as those by Case et al. (1999), Mott and Untener (2016), Seed (2001), Hibbeler (2016), Beer et al. (2014), and Goodno and Gere (2017).

14.1.1 Classification of pressure vessels

For the purposes of design and analysis, pressure vessels are subdivided into two classes, depending on the ratio of the wall thickness to vessel diameter: thin-walled vessels, with a thickness ratio of less than 1:10, and thick-walled above this ratio.

The principal stresses (see Section 14.3.1) acting at a point in the wall of a vessel, due to a pressure load, are shown in Fig. 14.1. If the wall is thin, the radial stress σ_3 will be small and can be neglected in comparison with the other stresses, and the longitudinal and circumferential stresses σ_1 and σ_2 can be taken as constant over the wall thickness. In a thick wall, the magnitude of the radial stress will be significant, and the circumferential stress will vary across the wall. The majority of the vessels used in the chemical and allied industries are classified as thin-walled vessels. Thick-walled vessels are used for high pressures and are discussed in Section 14.14.

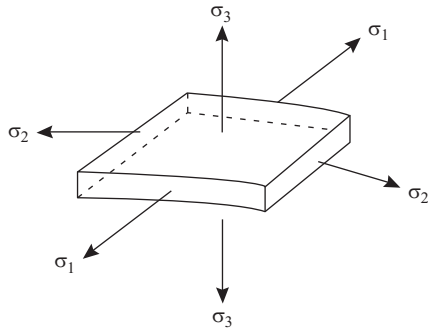


FIG. 14.1 Principal stresses in pressure-vessel wall.

14.2 Pressure vessel codes and standards

In all the major industrialized countries, the design and fabrication of pressure vessels are covered by national standards and codes of practice. In most countries it is a legal requirement that pressure vessels must be designed, constructed, and tested in accordance with part or all of the design code. The primary purpose of the design codes is to establish rules of safety relating to the pressure integrity of vessels and provide guidance on design, materials of construction, fabrication, inspection, and testing. They form a basis of agreement between the manufacturer and customer and the customer's insurance company.

The standard used in North America (and most commonly referenced internationally) is the ASME Boiler and Pressure Vessel Code (the ASME BPV Code). The 12 sections of the ASME BPV Code are listed in Table 14.1. Most chemical plant and refinery vessels fall within the scope of Section VIII of the ASME BPV Code. Section VIII contains three subdivisions:

Division 1: Contains general rules and is most commonly followed, particularly for low-pressure vessels.
Division 2: Contains alternative rules that are more restrictive on materials, design temperatures, design details, fabrication methods, and inspection but allow higher design stresses and hence thinner vessel walls. Division 2 rules are usually chosen for large, high-pressure vessels where the savings in metal cost and fabrication complexity offset the higher engineering and construction costs.
Division 3: Contains alternative rules intended for vessels with design pressures greater than 10,000 psig. It does not establish a maximum pressure for vessels designed in accordance with Division 1 or Division 2, but provides alternative rules that can be followed for thicker-walled vessels.

In the following sections reference will normally be made to the BPV Code Sec. VIII D.1. The scope of the BPV Code Sec. VIII D.1 covers vessels made from iron, steels, and nonferrous metals. It specifically excludes:

1. Vessels within the scope of other sections of the BPV code. For example, power boilers (Sec. I), fiber-reinforced plastic vessels (Sec. X), and transport tanks (Sec. XIII).
2. Fired process tubular heaters.
3. Pressure containers that are integral parts of rotating or reciprocating devices, such as pumps, compressors, turbines, or engines.
4. Piping systems (which are covered by ASME B31.3—see Chapter 20).
5. Piping components and accessories such as valves, strainers, in-line mixers, and spargers.
6. Vessels containing water at less than 300 psi (2 MPa) and less than 210 °F (99 °C).
7. Hot water storage tanks heated by steam with heat rate less than 0.2 MMBTU/h (58.6 kW), water temperature less than 210 °F (99 °C), and volume less than 120 gal (450 liters).
8. Vessels having internal pressure less than 15 psi (100 kPa) or greater than 3000 psi (20 MPa).
9. Vessels of internal diameter or height less than 6 in (152 mm).
10. Pressure vessels for human occupancy.

TABLE 14.1 The 2004 ASME Boiler and Pressure Vessel Code

SECTIONS	
I	Rules for construction of power boilers
II	Materials
	Part A Ferrous metal specifications
	Part B Nonferrous metal specifications
	Part C Specifications for welding rods, electrodes, and filler metals
	Part D Properties (customary or metric versions)
III	Nuclear power plant components
	NCA General requirements
	Division 1
	Division 2 Code for concrete containments
	Division 3 Containments for transport and storage of spent nuclear fuel and high level radioactive material and waste
IV	Rules for construction of heating boilers
V	Nondestructive examination
VI	Recommended rules for the care and operation of heating boilers

Continued

TABLE 14.1 The 2004 ASME Boiler and Pressure Vessel Code—cont'd

VII	Recommended guidelines for the care of power boilers
VIII	Rules for the construction of pressure vessels
	Division 1
	Division 2 Alternative rules
	Division 3 Alternative rules for the construction of high pressure vessels
IX	Welding and brazing qualifications
X	Fiber-reinforced plastic vessels
XI	Rules for in service inspection of nuclear power plant components
XII	Rules for construction and continued service of transport tanks

The ASME BPV Code can be ordered from ASME and is also available online (for example at ihsmarkit.com). The most recent edition of the code should always be consulted during detailed design.

In addition to the BPV Code Sec. VIII, the process design engineer will frequently need to consult Section II Part D, which lists maximum allowable stress values under Sec. VIII D.1 and D.2, as well as other materials properties. Comprehensive reviews of the ASME code are given by Ellenberger et al. (2004), Farr and Jawad (2010), and Yokell (1986); see also Green and Southard (2018).

In the European Union the design, manufacture, and use of pressure systems is covered by the Pressure Equipment Directive (Council Directive 97/23/EC) whose use became mandatory in May 2002. European standard EN 13445 provides similar rules and guidelines to the ASME BPV Code. The design of fiber-reinforced plastic vessels is covered by European standard EN 13923. The European standards can be obtained from any of the European Union member country national standards agencies; for example, BS EN 13445 can be ordered from www.bsigroup.com. Where national codes are not available, the ASME or European codes would normally be used.

Information and guidance on the pressure vessel codes can be found on the Internet at ihsmarkit.com or www.bsigroup.com.

The national codes and standards dictate the minimum requirements and give general guidance for design and construction; any extension beyond the minimum code requirement will be determined by agreement between the manufacturer and customer.

The codes and standards are drawn up by committees of engineers experienced in vessel design and manufacturing techniques and are a blend of theory, experiment, and experience. They are periodically reviewed, and revisions are issued to keep abreast of developments in design, stress analysis, fabrication, and testing. The latest version of the appropriate national code or standard should always be consulted before undertaking the design of any pressure vessel.

Several commercial computer programs to aid in the design of vessels to the ASME code and other international codes are available. These programs will normally be used by the specialist mechanical engineers who carry out the detailed vessel design. Some examples include:

Pressure Vessel Suite (Computer Engineering, Inc.)
PVElite and CodeCalc (COADE, Inc.)
TEMA/ASME and COMPRESS (Codeware, Inc.)

14.3 Fundamentals of strength of materials

This section has been included to provide a basic understanding of the fundamental principles that underlie the design equations given in the sections that follow. The derivation of the equations is given in outline only. A detailed knowledge of the material in this section is not required for preliminary vessel design, but the equations derived here will be referenced and applied in subsequent sections. A full discussion of the topics covered can be found in any text on the "strength of materials" (mechanics of solids).

14.3.1 Principal stresses

The state of stress at a point in a structural member under a complex system of loading is described by the magnitude and direction of the principal stresses. The principal stresses are the maximum values of the normal stresses at

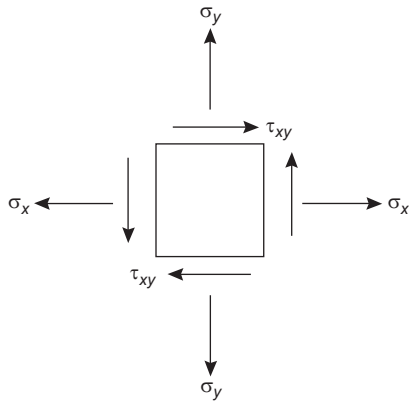


FIG. 14.2 Two-dimensional stress system.

the point, which act on planes on which the shear stress is zero. In a two-dimensional stress system (Fig. 14.2), the principal stresses at any point are related to the normal stresses in the x and y directions σ_x and σ_y and the shear stress τ_{xy} at the point by the following equation:

$$\text{Principal stresses, } \sigma_1,\ \sigma_2 = \frac{1}{2}(\sigma_y + \sigma_x) \pm \frac{1}{2}\sqrt{\left[(\sigma_y - \sigma_x)^2 + 4\tau_{xy}^2\right]} \tag{14.1}$$

The maximum shear stress at the point is equal to half the algebraic difference between the principal stresses:

$$\text{Maximum shear stress} = \frac{1}{2}(\sigma_1 - \sigma_2) \tag{14.2}$$

Compressive stresses are conventionally taken as negative; tensile as positive.

14.3.2 Theories of failure

The failure of a simple structural element under unidirectional stress (tensile or compressive) is easy to relate to the tensile strength of the material, as determined in a standard tensile test, but for components subjected to combined stresses (normal and shear stress), the position is not so simple, and several theories of failure have been proposed. The three theories most commonly used are described next.

Maximum principal stress theory postulates that a member will fail when one of the principal stresses reaches the failure value in simple tension, σ_e. The failure point in a simple tension is taken as the yield-point stress, or the tensile strength of the material, divided by a suitable factor of safety.

Maximum shear stress theory postulates that failure will occur in a complex stress system when the maximum shear stress reaches the value of the shear stress at failure in simple tension.

For a system of combined stresses, there are three shear stress maxima:

$$\tau_1 = \frac{\sigma_1 - \sigma_2}{2} \tag{14.3a}$$

$$\tau_2 = \frac{\sigma_2 - \sigma_3}{2} \tag{14.3b}$$

$$\tau_3 = \frac{\sigma_3 - \sigma_1}{2} \tag{14.3c}$$

In the tensile test,

$$\tau_e = \frac{\sigma_e}{2} \tag{14.4}$$

The maximum shear stress will depend on the sign of the principal stresses as well as their magnitude, and in a two-dimensional stress system, such as that in the wall of a thin-walled pressure vessel, the maximum value of the shear stress may be that given by putting $\sigma_3 = 0$ in Equations 14.3b and c.

The maximum shear stress theory is often called Tresca's, or Guest's, theory.

Maximum strain energy theory postulates that failure will occur in a complex stress system when the total strain energy per unit volume reaches the value at which failure occurs in simple tension.

The maximum shear-stress theory has been found to be suitable for predicting the failure of ductile materials under complex loading and is the criterion normally used in pressure vessel design.

14.3.3 Elastic stability

Under certain loading conditions, failure of a structure can occur not through gross yielding or plastic failure, but by buckling or wrinkling. Buckling leads to a gross and sudden change of shape of the structure, unlike failure by plastic yielding, where the structure retains the same basic shape. This mode of failure will occur when the structure is not elastically stable: when it lacks sufficient stiffness, or rigidity, to withstand the load. The stiffness of a structural member is dependent not on the basic strength of the material but on its elastic properties (E_Y and v) and the cross-sectional shape of the member.

The classic example of failure due to elastic instability is the buckling of tall thin columns (struts), which is described in any elementary text on the "strength of materials." For a structure that is likely to fail by buckling, there will be a certain critical value of load below which the structure is stable; if this value is exceeded, catastrophic failure through buckling can occur.

The walls of pressure vessels are usually relatively thin compared with the other dimensions and can fail by buckling under compressive loads. This is particularly important for tall, wide vessels such as distillation columns that can experience compressive loads from wind loads.

Elastic buckling is the decisive criterion in the design of thin-walled vessels under external pressure.

14.3.4 Secondary stresses

In the stress analysis of pressure vessels and pressure vessel components, stresses are classified as primary or secondary. Primary stresses can be defined as those stresses that are necessary to satisfy the conditions of static equilibrium. The membrane stresses induced by the applied pressure and the bending stresses due to wind loads are examples of primary stresses. Primary stresses are not self-limiting; if they exceed the yield point of the material, gross distortion, and in the extreme situation, failure of the vessel will occur.

Secondary stresses are those stresses that arise from the constraint of adjacent parts of the vessel. Secondary stresses are self-limiting; local yielding or slight distortion will satisfy the conditions causing the stress, and failure would not be expected to occur in one application of the loading. The "thermal stress" set up by the differential expansion of parts of the vessel, due to different temperatures or the use of different materials, is an example of a secondary stress. The discontinuity that occurs between the head and the cylindrical section of a vessel is a major source of secondary stress. If free, the dilation of the head would be different from that of the cylindrical section; they are constrained to the same dilation by the welded joint between the two parts. The induced bending moment and shear force due to the constraint give rise to secondary bending and shear stresses at the junction. The magnitude of these discontinuity stresses can be estimated by analogy with the behavior of beams on elastic foundations; see Hetenyi (1958) and Harvey (1974). The estimation of the stresses arising from discontinuities is covered in the books by Bednar (1990) and Jawad and Farr (2018). Other sources of secondary stresses are the constraints arising at flanges, supports, and the change of section due to reinforcement at a nozzle or opening (see Section 14.6).

Though secondary stresses do not affect the "bursting strength" of the vessel, they are an important consideration when the vessel is subject to repeated pressure loading. If local yielding has occurred, residual stress will remain when the pressure load is removed, and repeated pressure cycling can lead to fatigue failure.

14.4 General design considerations for pressure vessels

This section describes general pressure vessel design specifications, most of which would normally be specified by a process engineer.

14.4.1 Design pressure

A vessel must be designed to withstand the maximum pressure to which it is likely to be subjected in operation.

For vessels under internal pressure, the design pressure (sometimes called maximum allowable working pressure [MAWP]) is taken as the pressure at which the relief device is set. This will normally be 5% to 10% above the normal working pressure to avoid spurious operation during minor process upsets. For example, API STD 520 recommended practice sets a 10% margin between the normal operating pressure and the design pressure. When deciding the design pressure, the hydrostatic pressure in the base of the column should be added to the operating pressure, if significant.

Vessels subject to external pressure should be designed to resist the maximum differential pressure that is likely to occur in service. Vessels likely to be subjected to vacuum should be designed for a full negative pressure of 1 bar, unless fitted with an effective, and reliable, vacuum breaker.

14.4.2 Design temperature

The strength of metals decreases with increasing temperature (see Chapter 6), so the maximum allowable stress will depend on the material temperature. The maximum design temperature at which the maximum allowable stress is evaluated should be taken as the maximum working temperature of the material, with due allowance for any uncertainty involved in predicting vessel wall temperatures. Additional rules apply for welded vessels, as described in ASME BPV Code Sec. VIII D.1 part UW. The minimum design metal temperature (MDMT) should be taken as the lowest temperature expected in service. The designer should consider the lowest operating temperature, ambient temperature, auto-refrigeration, process upsets, and other sources of cooling in determining the minimum.

14.4.3 Materials

Pressure vessels are constructed from plain carbon steels, low- and high-alloy steels, other alloys, clad plate, and reinforced plastics.

Selection of a suitable material must take into account the suitability of the material for fabrication (particularly welding), as well as the compatibility of the material with the process environment; see Chapter 6.

The pressure vessel design codes and standards include lists of acceptable materials in accordance with the appropriate material standards. The ASME BPV Code Sec. II Part D gives maximum allowable stresses as a function of temperature and maximum temperatures permitted under Sections I, III, VIII, and XII of the BPV code for ferrous and nonferrous metals. The design of pressure vessels using reinforced plastics is described in ASME BPV Code Sec. X.

14.4.4 Maximum allowable stress (nominal design strength)

For design purposes, it is necessary to decide a value for the maximum allowable stress (nominal design strength) that can be accepted in the material of construction.

This is determined by applying a suitable safety factor to the maximum stress that the material could be expected to withstand without failure under standard test conditions. The safety factor allows for any uncertainty in the design methods, the loading, the quality of the materials, and the workmanship.

The basis for establishing the maximum allowable stress values in the ASME BPV Code is given in ASME BPV Code Sec. II Part D, Mandatory Appendix 1. At temperatures where creep and stress rupture strength do not govern the selection of stresses, the maximum allowable stress is the lowest of:

1. The specified minimum tensile strength at room temperature divided by 3.5
2. The tensile strength at temperature divided by 3.5
3. The specified minimum yield strength at room temperature divided by 1.5
4. The yield strength at temperature divided by 1.5

At temperatures where creep and stress rupture strength govern, the maximum allowable stress is the lowest of:

1. The average stress to produce a creep rate of 0.01%/1000 hr
2. F times the average stress to cause rupture at the end of 100,000 hr, where $F = 0.67$ for temperatures below 1500 °F (815 °C)—see the code for higher temperatures
3. 0.8 times the minimum stress to cause rupture after 100,000 hr

In some cases where short-time tensile properties govern and slightly greater deformation is acceptable, higher stress values are allowed under ASME BPV Code Sec. VIII D.1. These exceed 67% but do not exceed 90% of the yield strength at temperature. These cases are indicated with a note (G5) in the BPV Code tables. Use of these higher values can result in deformation and changes in the vessel dimensions. They are not recommended for flanges or other applications where changes in dimensions could lead to leaks or vessel malfunction.

The maximum allowable stress values for ASME BPV Code Sec. VIII D.1 are given in ASME BPV Code Sec II Part D Table 1A for ferrous metals and Table 1B for nonferrous metals. Maximum allowable stress values for Sec. VIII D.2 are given in Sec. II Part D Table 2A for ferrous metals and Table 2B for nonferrous metals. Different values are given for plate, tubes, castings, forgings, bar, pipe, and small sections, as well as for different grades of each metal.

Typical maximum allowable stress values for some common materials are shown in Table 14.2. These may be used for preliminary designs. The ASME BPV Code should be consulted for the values to be used for detailed vessel design.

TABLE 14.2 Typical maximum allowable stresses for plates under ASME BPV Code Sec. VIII D.1 (The appropriate material standards should be consulted for particular grades and plate thicknesses.)

Material	Grade	Min. tensile strength (ksi)	Min. yield strength (ksi)	Maximum temperature (°F)	Maximum allowable stress at temperature °F (ksi = 1000 psi)				
					100	300	500	700	900
Carbon steel	A285 Gr A	45	24	900	12.9	12.9	12.9	11.5	5.9
Killed carbon steel	A515 Gr 60	60	32	1000	17.1	17.1	17.1	14.3	5.9
Low-alloy steel 1¼ Cr, ½ Mo, Si	A387 Gr 22	60	30	1200	17.1	16.6	16.6	16.6	13.6
Stainless steel 13 Cr	410	65	30	1200	18.6	17.8	17.2	16.2	12.3
Stainless steel 18 Cr, 8 Ni	304	75	30	1500	20.0	15.0	12.9	11.7	10.8
Stainless steel 18 Cr, 10 Ni, Cb	347	75	30	1500	20.0	17.1	15.0	13.8	13.4
Stainless steel 18 Cr, 10 Ni, Ti	321	75	30	1500	20.0	16.5	14.3	13.0	12.3
Stainless steel 16 Cr, 12 Ni, 2 Mo	316	75	30	1500	20.0	15.6	13.3	12.1	11.5

Note:
1. The stress values for type 304 stainless steel are not the same as those given for stainless steel 304L in Table 7.8.
2. 1 ksi = 1000 psi = 6.8948 N/mm^2

14.4.5 Welded joint efficiency and construction categories

The strength of a welded joint will depend on the type of joint and the quality of the welding. The ASME BPV Code Sec. VIII D.1 defines four categories of weld (Part UW-3):

1. Longitudinal or spiral welds in the main shell, necks, or nozzles or circumferential welds connecting hemispherical heads to the main shell, necks, or nozzles.
2. Circumferential welds in the main shell, necks, or nozzles or connecting a formed head other than hemispherical.
3. Welds connecting flanges, tubesheets, or flat heads to the main shell, a formed head, neck, or nozzle.
4. Welds connecting communicating chambers or nozzles to the main shell, to heads, or to necks.

Details of the different types of welds used in pressure vessel construction are given in Section 14.11.

The soundness of welds is checked by visual inspection and by nondestructive testing (radiography).

The possible lower strength of a welded joint compared with the virgin plate is usually allowed for in design by multiplying the allowable design stress for the material by a joint efficiency E. The value of the joint efficiency used in design will depend on the type of joint and amount of radiography required by the design code. Typical values are shown in Table 14.3. A joint efficiency of 1.0 is only permitted for butt joints formed by double welding and subjected to full radiographic examination. Taking the factor as 1.0 implies that the joint is equally as strong as the virgin plate; this is achieved by radiographing the complete weld length and cutting out and remaking any defects. The use of lower joint efficiencies in design, though saving costs on radiography, will result in a thicker, heavier vessel, and the designer must balance any cost savings on inspection and fabrication against the increased cost of materials.

The ASME BPV Code Sec. VIII D.1 Part UW describes the requirements for pressure vessels fabricated by welding. Limiting plate thicknesses are specified for each type of weld with the exception of double-welded butt joints. Requirements for radiographic examination of welds are also specified. Section UW-13 of the code specifies the types of welds that can be used to attach heads and tubesheets to shells. Section UW-16 gives rules for attachment of nozzles to vessels.

The BPV Code should be consulted to determine the allowed joint types for a particular vessel. Any pressure vessel containing lethal substances will require full radiographic testing of all butt welds.

TABLE 14.3 Maximum allowable joint efficiency

		Degree of radiographic examination		
Joint description	**Joint category**	**Full**	**Spot**	**None**
Double-welded butt joint or equivalent	A, B, C, D	1.0	0.85	0.70
Single-welded butt joint with backing strip	A, B, C, D	0.9	0.8	0.65
Single-welded butt joint without backing strip	A, B, C	NA	NA	0.60
Double full-fillet lap joint	A, B, C	NA	NA	0.55
Single full-fillet lap joint with plug welds	B, C	NA	NA	0.50
Single full-fillet lap joint without plug welds	A, B	NA	NA	0.45

14.4.6 Corrosion allowance

The "corrosion allowance" is the additional thickness of metal added to allow for material lost by corrosion and erosion or scaling (see Chapter 6). The ASME BPV Code Sec. VIII D.1 states that the vessel user shall specify corrosion allowances (Part UG-25). Minimum wall thicknesses calculated using the rules given in the code are in the fully corroded condition (Part UG-16). Corrosion is a complex phenomenon, and it is not possible to give specific rules for the estimation of the corrosion allowance required for all circumstances. The allowance should be based on experience with the material of construction under similar service conditions to those for the proposed design. For carbon and low-alloy steels, where severe corrosion is not expected, a minimum allowance of 2.0 mm should be used; where more severe conditions are anticipated, this should be increased to 4.0 mm. Most design codes and standards specify a minimum allowance of 1.0 mm, but under the ASME BPV Code Sec. VIII no corrosion allowance is needed when past experience indicates that corrosion is only superficial or does not occur.

14.4.7 Design loads

A structure must be designed to resist gross plastic deformation and collapse under all the conditions of loading. The loads to which a process vessel will be subject in service are listed next. They can be classified as major loads that must always be considered in vessel design and subsidiary loads. Formal stress analysis to determine the effect of the subsidiary loads is only required in the codes and standards where it is not possible to demonstrate the adequacy of the proposed design by other means, such as by comparison with the known behavior of existing vessels.

Major loads

1. Design pressure, including any significant static head of liquid
2. Maximum weight of the vessel and contents under operating conditions
3. Maximum weight of the vessel and contents under the hydraulic test conditions
4. Wind loads
5. Earthquake (seismic) loads
6. Loads supported by, or reacting on, the vessel

Subsidiary loads

1. Local stresses caused by supports, internal structures, and connecting pipes
2. Shock loads caused by water hammer or by surging of the vessel contents
3. Bending moments caused by eccentricity of the center of the working pressure relative to the neutral axis of the vessel
4. Stresses due to temperature differences and differences in the coefficient of expansion of materials
5. Loads caused by fluctuations in temperature and pressure

A vessel will not be subject to all these loads simultaneously. The designer must determine what combination of possible loads gives the worst situation (the "governing case") and design for that loading condition.

14.4.8 Minimum practical wall thickness

There will be a minimum wall thickness required to ensure that any vessel is sufficiently rigid to withstand its own weight, and any incidental loads. The ASME BPV Code Sec. VIII D.1 specifies a minimum wall thickness of {1/16} in (1.5 mm), not including corrosion allowance, and regardless of vessel dimensions and material of construction. As a general guide, the wall thickness of any vessel should not be less than the values given here; the values include a corrosion allowance of 2 mm:

Vessel diameter (m)	Minimum thickness (mm)
1	5
1–2	7
2–2.5	9
2.5–3.0	10
3.0–3.5	12

14.5 The design of thin-walled vessels under internal pressure

14.5.1 Cylinders and spherical shells

The walls of thin vessels can be considered to be "membranes"; supporting loads without significant bending or shear stresses; similar to the walls of a balloon. The analysis of the membrane stresses induced in the wall by internal pressure gives a basis for determining the minimum wall thickness required for vessel shells. The actual thickness required will also depend on the stresses arising from the other loads to which the vessel is subjected.

For a cylindrical shell, the stresses in the walls can be determined from simple force balances, as the wall stresses must balance the forces due to pressure. If we consider a horizontal section through the vessel (Fig. 14.3a), then the force due to pressure on the cross-section is:

$$F_L = \frac{P_i \pi D^2}{4} \tag{14.5}$$

Where P_i = internal pressure
D = mean diameter
F_L = force in longitudinal direction

This force must be balanced by the longitudinal stress in the wall of the cylinder, which acts only on the sectioned area of the wall:

$$F_L = \sigma_L \, \pi \, D \, t \tag{14.6}$$

Where σ_L = longitudinal stress
t = wall thickness

Equating Equations 14.5 and 14.6:

$$\sigma_L = \frac{P_i D}{4t} \tag{14.7}$$

Similarly, if we consider a vertical section in an infinite cylinder (Fig. 14.3b), the force due to pressure on a vertical section of length L is:

$$F_v = P_i \, D \, L \tag{14.8}$$

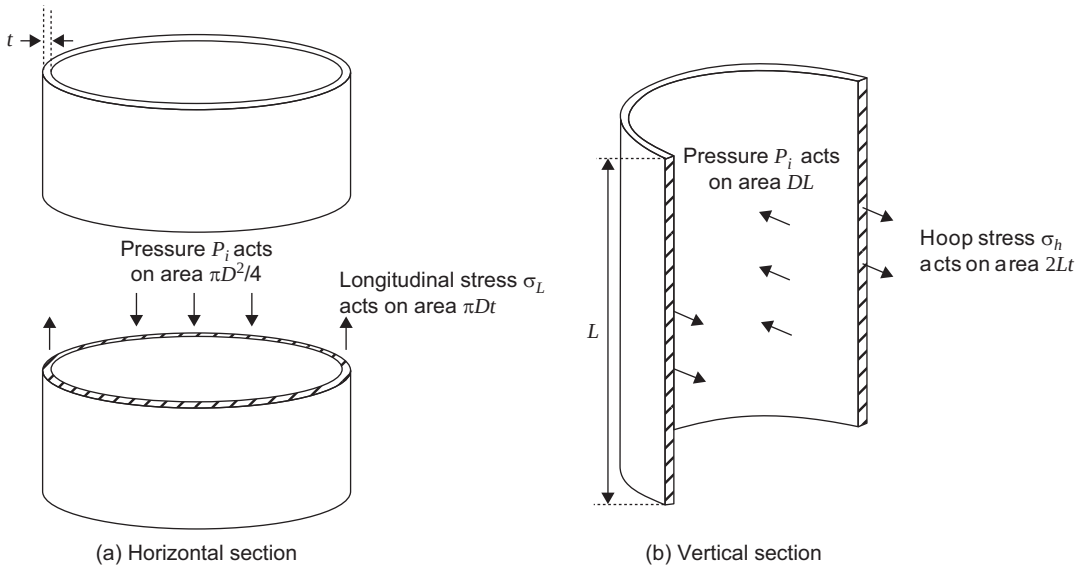


FIG. 14.3 Stresses in the walls of cylindrical vessels due to internal pressure.

Where F_v = force in horizontal direction
L = length

This force is balanced by the circumferential or hoop stress in the wall of the cylinder, which acts only on the sectioned area of the cylinder:

$$F_v = \sigma_h (2\,L\,t) \tag{14.9}$$

Where σ_h = hoop stress
Equating Equations 14.8 and 14.9:

$$\sigma_h = \frac{P_i D}{2t} \tag{14.10}$$

The minimum wall thickness that is required to contain the internal pressure can be determined using Equations 14.7 and 14.10.

If D_i is internal diameter and t the minimum thickness required, the mean diameter will be $(D_i + t)$; substituting this for D in Equation 14.10 gives:

$$t = \frac{P_i(D_i + t)}{2S}$$

where S is the maximum allowable stress and P_i the internal pressure. Rearranging gives:

$$t = \frac{P_i\,D_i}{2S - P_i} \tag{14.11}$$

If we allow for the welded joint efficiency, E, this becomes:

$$t = \frac{P_i\,D_i}{2SE - P_i} \tag{14.12}$$

The equation specified by the ASME BPV Code (Sec. VIII D.1 Part UG-27) is:

$$t = \frac{P_i\,D_i}{2SE - 1.2P_i} \tag{14.13}$$

This differs slightly from Equation 14.12, as it is derived from the formula for thick-walled vessels.

Similarly, for longitudinal stress the code specifies:

$$t = \frac{P_i\,D_i}{4SE + 0.8P_i} \tag{14.14}$$

The ASME BPV Code specifies that the minimum thickness shall be the greater value determined from Equations 14.13 and 14.14. If these equations are rearranged and used to calculate the MAWP for a vessel of a given thickness, then the MAWP is the lower value predicted by the two equations.

For a spherical shell, the code specifies:

$$t = \frac{P_i\,D_i}{4SE - 0.4P_i} \tag{14.15}$$

Any consistent set of units can be used for Equations 14.13 to 14.15.

14.5.2 Heads and closures

The ends of a cylindrical vessel are closed by heads of various shapes. The principal types used are:

1. Flat plates and formed flat heads; Fig. 14.4
2. Hemispherical heads; Fig. 14.5(a)
3. Ellipsoidal heads; Fig. 14.5(b)
4. Torispherical heads; Fig. 14.5(c)

Hemispherical, ellipsoidal, and torispherical heads are collectively referred to as domed heads. They are formed by pressing or spinning; large diameters are fabricated from formed sections. Torispherical heads are often referred

to as dished ends. The preferred proportions of domed heads are given in the standards and codes. Vessel heads can be made in any size, but standard sizes (which come in 6-inch increments) will usually be cheaper.

Choice of closure

Flat plates are used as covers for manways and as the channel covers of heat exchangers. Formed flat ends, known as "flange-only" ends, are manufactured by turning over a flange with a small radius on a flat plate (see Fig. 14.4a). The corner radius reduces the abrupt change of shape at the junction with the cylindrical section, which reduces the local stresses to some extent. "Flange-only" heads are the cheapest type of formed head to manufacture, but their use is limited to low-pressure and small-diameter vessels.

Standard torispherical heads (dished ends) are the most commonly used end closure for vessels up to operating pressures of 15 bar. They can be used for higher pressures, but above 10 bar their cost should be compared with that of an equivalent ellipsoidal head. Above 15 bar an ellipsoidal head will usually prove to be the most economical closure to use.

A hemispherical head is the strongest shape, capable of resisting about twice the pressure of a torispherical head of the same thickness. The cost of forming a hemispherical head will, however, be higher than that for a shallow torispherical head. Hemispherical heads are used for high pressures.

14.5.3 Design of flat ends

Though the fabrication cost is low, flat ends are not a structurally efficient form, and very thick plates would be required for high pressures or large diameters.

The design equations used to determine the thickness of flat ends are based on the analysis of stresses in flat plates. The thickness required will depend on the degree of constraint at the plate periphery.

The ASME BPV Code specifies the minimum thickness as:

$$t = D_e\sqrt{\frac{C\,P_i}{S\,E}} \tag{14.16}$$

where C = a design constant, dependent on the edge constraint
D_e = nominal plate diameter
S = maximum allowable stress
E = joint efficiency

Any consistent set of units can be used.

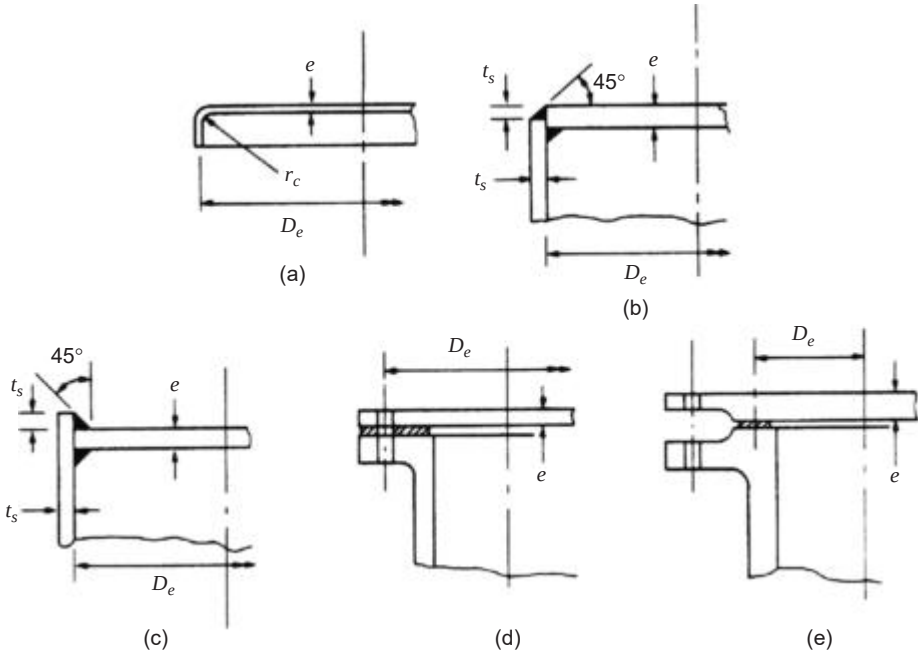


FIG. 14.4 Flat-end closures. (a) Flanged plate. (b) Welded plate. (c) Welded plate. (d) Bolted cover. (e) Bolted cover.

Values for the design constant C and the nominal plate diameter D_e are given in the ASME BPV Code for various arrangements of flat end closures (Sec. VIII D.1 Part UG-34).

Some typical values of the design constant and nominal diameter for the designs shown in Fig. 14.4 are given here. For detailed design, the ASME BPV Code should be consulted.

(a) Flanged-only end, $C = 0.17$ if corner radius is not more than $3t$; otherwise, $C = 0.1$; D_e is equal to D_i.

(b and c) Plates welded to the end of the shell with a fillet weld, angle of fillet 45 degrees and weld depth 70% of the thickness of the shell, $C = 0.33\ t/t_s$, where t_s is the shell thickness. $D_e = D_i$.

(d) Bolted cover with a full face gasket (see Section 14.10), $C = 0.25$ and D_e is the bolt circle diameter (the diameter of a circle connecting the centers of the bolt holes).

(e) Bolted end cover with a narrow-face gasket, $C = 0.3$ and D_e should be taken as the mean diameter of the gasket.

14.5.4 Design of domed ends

Design equations and charts for the various types of domed heads are given in the ASME BPV Code and should be used for detailed design. The code covers both unpierced and pierced heads. Pierced heads are those with openings or connections. The head thickness must be increased to compensate for the weakening effect of the holes where the opening or branch is not locally reinforced (see Section 14.6).

For convenience, simplified design equations are given in this section. These are suitable for the preliminary sizing of unpierced heads and for heads with fully compensated openings or branches.

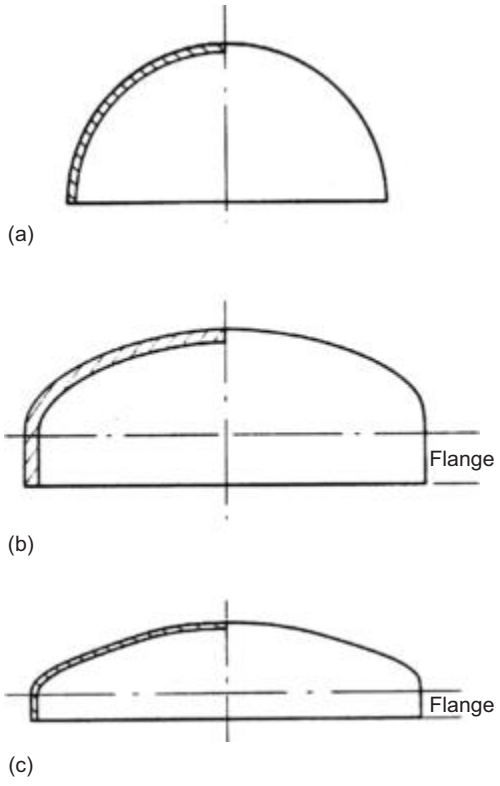


FIG. 14.5 Domed heads. (a) Hemispherical. (b) Ellipsoidal. (c) Torispherical.

Hemispherical heads

For equal stress in the cylindrical section and hemispherical head of a vessel, the thickness of the head need only be half that of the cylinder; however, as the dilation of the two parts would then be different, discontinuity stresses would be set up at the head and cylinder junction. For no difference in dilation between the two parts (equal diametrical strain), it can be shown that for steels (Poisson ratio = 0.3), the ratio of the hemispherical head thickness to cylinder thickness should be 7/17. However, the stress in the head would then be greater than that in the cylindrical section, and the optimum thickness ratio is normally taken as 0.6; see Brownell and Young (1959).

In the ASME BPV Code Sec. VIII D.1, the equation specified is the same as for a spherical shell:

$$t = \frac{P_i D_i}{4SE - 0.4P_i} \tag{14.17}$$

Ellipsoidal heads

Most standard ellipsoidal heads are manufactured with a major and minor axis ratio of 2:1. For this ratio, the following equation can be used to calculate the minimum thickness required (ASME BPV Code Sec. VIII D.1 Part UG-32):

$$t = \frac{P_i D_i}{2SE - 0.2P_i} \tag{14.18}$$

Torispherical heads

A torispherical shape is formed from part of a torus and part of a sphere (Fig. 14.5c). The shape is close to that of an ellipse but is easier and cheaper to fabricate.

In Fig. 14.6, R_k is the knuckle radius (the radius of the torus) and R_c the crown radius (the radius of the sphere). The stress will be higher in the torus section than the spherical section.

There are two junctions in a torispherical end closure: that between the cylindrical section and the head and that at the junction of the crown and the knuckle radii. The bending and shear stresses caused by the differential dilation that will occur at these points must be taken into account in the design of the heads. The ASME BPV Code gives the design equation (Sec. VIII D.1 Part UG-32):

$$t = \frac{0.885 P_i R_c}{SE - 0.1P_i} \tag{14.19}$$

The ratio of the knuckle to crown radii should not be less than 0.06, to avoid buckling; and the crown radius should not be greater than the diameter of the cylindrical section. Any consistent set of units can be used with Equations 14.17 to 14.19. For formed heads (no welds or joints in the head), the joint efficiency E is taken as 1.0.

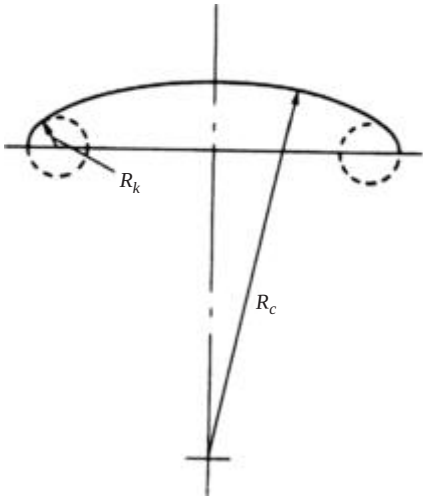


FIG. 14.6 Torisphere.

Flanges (skirts) on domed heads

Formed domed heads are made with a short, straight cylindrical section, called a flange or skirt (Fig. 14.5). This ensures that the weld line is away from the point of discontinuity between the head and the cylindrical section of the vessel.

14.5.5 Conical sections and end closures

Conical sections (reducers) are used to make a gradual reduction in diameter from one cylindrical section to another of smaller diameter.

Conical ends are used to facilitate the smooth flow and removal of solids from process equipment such as hoppers, spray dryers, and crystallizers.

The thickness required at any point on a cone is related to the diameter by the following expression:

$$t = \frac{P_i D_c}{2SE - P_i} \cdot \frac{1}{\cos \alpha} \tag{14.20}$$

where D_c = the diameter of the cone at the point
α = half the cone apex angle

The equation given in the ASME BPV Code is:

$$t = \frac{P_i D_i}{2 \cos \alpha \ (SE - 0.6P_i)} \tag{14.21}$$

This equation will only apply at points away from the cone-to-cylinder junction. Bending and shear stresses will be caused by the different dilations of the conical and cylindrical sections. A formed section would normally be used for the transition between a cylindrical section and conical section; except for vessels operating at low pressures, or under hydrostatic pressure only. The transition section would be made thicker than the conical or cylindrical section and formed with a knuckle radius to reduce the stress concentration at the transition (Fig. 14.7). The thickness for the conical section away from the transition can be calculated from Equation 14.21.

The code should be consulted for details of how to size the knuckle zone.

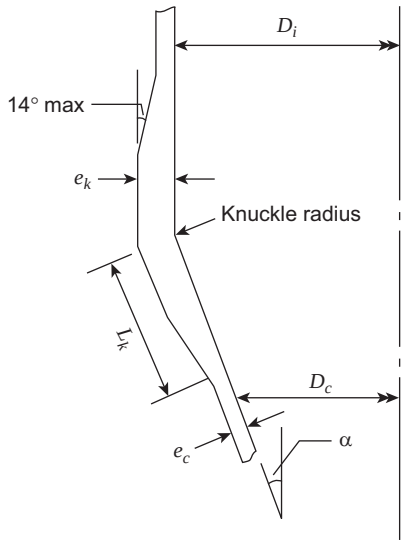
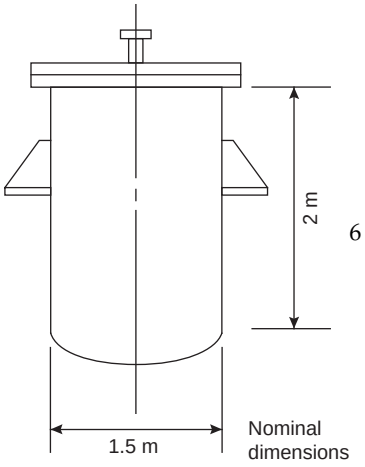


FIG. 14.7 Conical transition section.

Example 14.1

Estimate the thickness required for the component parts of the vessel shown in the diagram. The vessel is to operate at a pressure of 14 bar (absolute) and temperature of 260 °C. The material of construction will be plain carbon steel. Welds will be fully radiographed. A corrosion allowance of 2 mm should be used.



Solution

Design pressure, take as 10% above operating gauge pressure:

$$= (14 - 1) \times 1.1$$
$$= 14.3 \text{ bar}$$
$$= 1.43 \text{ N/mm}^2$$

Design temperature 260 °C (500 °F).
From Table 14.2, maximum allowable stress $= 12.9 \times 10^3$ psi $= 88.9$ N/mm^2.

Cylindrical section

$$t = \frac{1.43 \times 1.5 \times 10^3}{(2 \times 89 \times 1) - (1.2 \times 1.43)} = 12.2 \text{ mm} \tag{14.13}$$

$$\text{add corrosion allowance} \quad 12.2 + 2 = 14.2 \text{ mm}$$

$$\text{say} \quad \underline{15 \text{ mm plate}} \quad \text{or} \quad \underline{9/16 \text{ inch plate}}$$

Domed head

1. Try a standard dished head (torisphere):

crown radius $R_c = D_i = 1.5$ m
knuckle radius $= 6\%\ R_c = 0.09$ m

A head of this size would be formed by pressing: no joints, so $E = 1$.

$$t = \frac{0.885 \times 1.43 \times 1.5 \times 10^3}{(89 \times 1) - (0.1 \times 1.43)} = \underline{\underline{21.4 \text{ mm}}} \tag{14.19}$$

2. Try a "standard" ellipsoidal head, ratio major: minor axes = 2:1

$$t = \frac{1.43 \times 1.5 \times 10^3}{(2 \times 89 \times 1) - (0.2 \times 1.43)} = \underline{\underline{12.1 \text{ mm}}} \tag{14.18}$$

So an ellipsoidal head would probably be the most economical. Take as same thickness as wall 15 mm or 9/16 inch.

Flat head

Use a full face gasket $C = 0.25$

D_e = bolt circle diameter, take as approx. 1.7 m.

$$t = 1.7 \times 10^3 \sqrt{\frac{0.25 \times 1.43}{89 \times 1}} = \underline{\underline{107.7 \text{ mm}}} \tag{14.16}$$

Add corrosion allowance and round off to $\underline{\underline{111 \text{ mm}}}$ (4⅜ in).

This shows the inefficiency of a flat cover. It would be better to use a flanged domed head.

14.6 Compensation for openings and branches

All process vessels will have openings for connections, manways, and instrument fittings. The presence of an opening weakens the shell and gives rise to stress concentrations. The stress at the edge of a hole will be considerably higher than the average stress in the surrounding plate. To compensate for the effect of an opening, the wall thickness is increased in the region adjacent to the opening. Sufficient reinforcement must be provided to compensate for the weakening effect of the opening without significantly altering the general dilation pattern of the vessel at the opening. Overreinforcement will reduce the flexibility of the wall, causing a "hard spot," and giving rise to secondary stresses; typical arrangements are shown in Fig. 14.8.

The simplest method of providing compensation is to weld a pad or collar around the opening (see Fig. 14.8a). The outer diameter of the pad is usually between 1½ and 2 times the diameter of the hole or branch. This method, however, does not give the best disposition of the reinforcing material about the opening, and in some circumstances high thermal stress can arise due to the poor thermal conductivity of the pad-to-shell junction.

At a branch, the reinforcement required can be provided, with or without a pad, by allowing the branch to protrude into the vessel (see Fig. 14.8b). This arrangement should be used with caution for process vessels, as the protrusion will act as a trap for crud, and crevices are created in which localized corrosion can occur. Forged reinforcing rings (see Fig. 14.8c) provide the most effective method of compensation, but are expensive. They would be used for any large openings and branches in vessels operating under severe conditions.

The rules for calculating the minimum amount of reinforcement required are complex. For design purposes, consult the ASME BPV Code Sec. VIII D.1 Part UG-37.

14.7 Design of vessels subject to external pressure

Two types of process vessels are likely to be subjected to external pressure: those operated under vacuum, where the maximum pressure will be 1 bar (1 atm); and jacketed vessels, where the inner vessel will be under the jacket pressure. For jacketed vessels, the maximum pressure difference should be taken as the full jacket pressure, as a situation may arise in which the pressure in the inner vessel is lost. Thin-walled vessels subject to external pressure are vulnerable to failure through elastic instability (buckling), and it is this mode of failure that determines the wall thickness required.

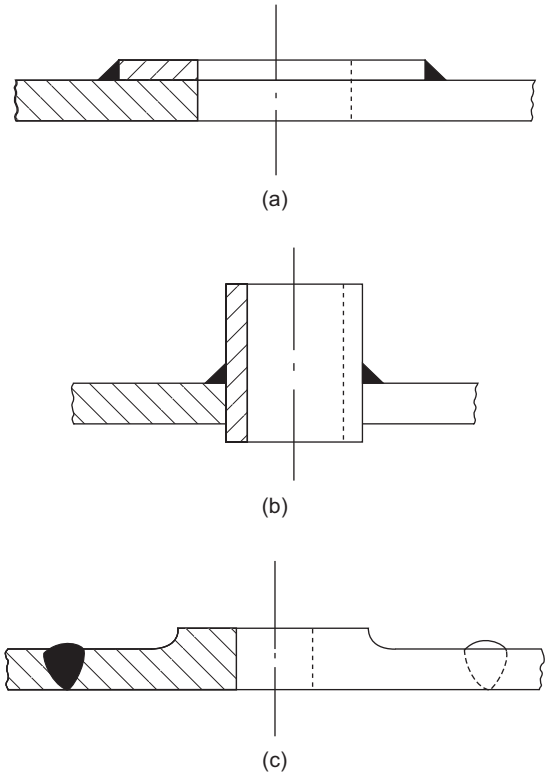


FIG. 14.8 Types of compensation for openings. (a) Welded pad. (b) Inset nozzle. (c) Forged ring.

The method recommended by the BPV Code for vessels subject to compressive stresses is substantially more complex than the method used for tensile stresses and takes into account the fact that the maximum allowable stress in compression is different from that in tension. The ASME BPV Code Sec. VIII D.1 Part UG-28 should be consulted for the approved method for detailed design of cylindrical vessels subject to external pressure. For detailed design of hemispherical vessel heads subject to external pressure, the method given in ASME BPV Code Sec. VIII D.1 Part UG-33 must be followed. Design methods for different shaped heads under external pressure are also given in the standards and codes.

Vessels that are subject to external pressure are often reinforced with internal stiffening rings. Methods for sizing the stiffening rings and determining their spacing are given in the BPV Code.

14.8 Design of vessels subject to combined loading

Pressure vessels are subjected to other loads in addition to pressure (see Section 14.4.7) and must be designed to withstand the worst combination of loading without failure. It is not practical to give an explicit relationship for the vessel thickness to resist combined loads. A trial thickness must be assumed (based on that calculated for pressure alone) and the resultant stress from all loads determined to ensure that the maximum allowable stress intensity is not exceeded at any point. When combined loads are analyzed, the maximum compressive stress must be considered, as well as the maximum tensile stress. The maximum allowable stress in compression is different from the maximum allowable stress in tension and is determined using the method given in ASME BPV Code Sec. VIII D.1 Part UG-23.

The main sources of load to consider are:

1. Pressure
2. Dead weight of vessel and contents

3. Wind
4. Earthquake (seismic)
5. External loads imposed by piping and attached equipment

The primary stresses arising from these loads are considered in the following paragraphs, for cylindrical vessels (Fig. 14.9).

Primary stresses

1. The longitudinal and circumferential stresses due to pressure (internal or external) are given by:

$$\sigma_L = \frac{PD_i}{4t} \tag{14.7}$$

$$\sigma_h = \frac{PD_i}{2t} \tag{14.10}$$

2. The direct stress σ_w due to the weight of the vessel, its contents, and any attachments. The stress will be tensile (positive) for points below the plane of the vessel supports and compressive (negative) for points above the supports (Fig. 14.10). The dead-weight stress will normally only be significant, compared with the magnitude of the other stresses, in tall vessels.

$$\sigma_w = \frac{W_z}{\pi(D_i + t)t} \tag{14.22}$$

where W_z is the total weight that is supported by the vessel wall at the plane considered (see Section 14.8.1).

3. Bending stresses resulting from the bending moments to which the vessel is subjected. Bending moments will be caused by the following loading conditions:
   a. The wind loads on tall self-supported vessels (Section 14.8.2)
   b. Seismic (earthquake) loads on tall vessels (Section 14.8.3)
   c. The dead weight and wind loads on piping and equipment that are attached to the vessel but offset from the vessel center line (Section 14.8.4)
   d. For horizontal vessels with saddle supports, from the disposition of dead-weight load (see Section 14.9.1)

   The bending stresses will be compressive or tensile, depending on location, and are given by:

$$\sigma_b = \pm \frac{M}{I_v}\left(\frac{D_i}{2} + t\right) \tag{14.23}$$

where M is the total bending moment at the plane being considered and I_v the second moment of area of the vessel about the plane of bending.

$$I_v = \frac{\pi}{64}\left(D_o^4 - D_i^4\right) \tag{14.24}$$

4. Torsional shear stresses τ resulting from torque caused by loads offset from the vessel axis. These loads will normally be small and need not be considered in preliminary vessel designs.

   The torsional shear stress is given by:

$$\tau = \frac{T}{I_p}\left(\frac{D_i}{2} + t\right) \tag{14.25}$$

where T = the applied torque

I_p = polar second moment of area $I_v = (\pi/32)\left(D_o^4 - D_i^4\right)$

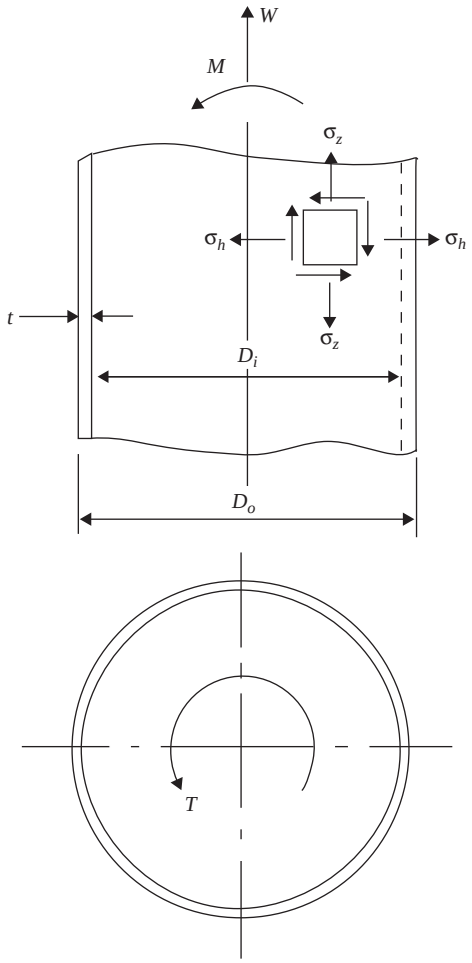


FIG. 14.9 Stresses in a cylindrical shell under combined loading.

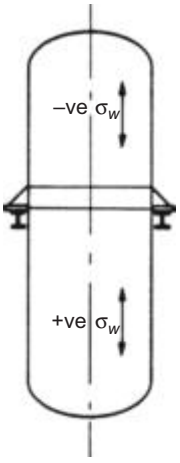


FIG. 14.10 Stresses due to dead-weight loads.

Principal stresses

The principal stresses will be given by:

$$\sigma_1 = \frac{1}{2}\left[\sigma_h + \sigma_z + \sqrt{(\sigma_h - \sigma_z)^2 + 4\tau^2}\right] \tag{14.26}$$

$$\sigma_2 = \frac{1}{2}\left[\sigma_h + \sigma_z - \sqrt{(\sigma_h - \sigma_z)^2 + 4\tau^2}\right] \tag{14.27}$$

where

σ_z = total longitudinal stress
$= \sigma_L + \sigma_w \pm \sigma_b$
σ_w should be counted as positive if tension and negative if compressive.
τ is not usually significant.

The third principal stress, that in the radial direction σ_3, will usually be negligible for thin-walled vessels (see Section 14.1.1). As an approximation, it can be taken as equal to one-half the pressure loading

$$\sigma_3 = 0.5P \tag{14.28}$$

σ_3 will be compressive (negative).

Allowable stress intensity

The maximum intensity of stress allowed will depend on the particular theory of failure adopted in the design method (see Section 14.3.2). The maximum shear-stress theory is normally used for pressure vessel design.

Using this criterion, the maximum stress intensity at any point is taken for design purposes as the numerically greatest value of the following:

$$(\sigma_1 - \sigma_2)$$

$$(\sigma_1 - \sigma_3)$$

$$(\sigma_2 - \sigma_3)$$

The vessel wall thickness must be sufficient to ensure the maximum stress intensity does not exceed the maximum allowable stress (nominal design strength) for the material of construction at any point. The ASME BPV Code Sec. II Part D should be consulted for the maximum allowable stress values in tension or in compression.

Compressive stresses and elastic stability

Under conditions where the resultant axial stress σ_z due to the combined loading is compressive, the vessel may fail by elastic instability (buckling) (see Section 14.3.3). Failure can occur in a thin-walled process column under an axial compressive load by buckling of the complete vessel, as with a strut (Euler buckling); or by local buckling, or wrinkling, of the shell plates. Local buckling will normally occur at a stress lower than that required to buckle the complete vessel. A column design must be checked to ensure that the maximum value of the resultant axial stress does not exceed the critical value at which buckling will occur.

For a curved plate subjected to an axial compressive load, the critical buckling stress σ_c is given by (see Timoshenko & Gere, 2009):

$$\sigma_c = \frac{E_Y}{\sqrt{3(1 - \nu^2)}}\left(\frac{t}{R_p}\right) \tag{14.29}$$

where R_p is the radius of curvature.

Taking Poisson's ratio as 0.3 gives:

$$\sigma_c = 0.60\, E_Y \left(\frac{t}{R_p}\right) \tag{14.30}$$

By applying a suitable factor of safety, Equation 14.30 can be used to predict the maximum allowable compressive stress to avoid failure by buckling. A large factor of safety is required, as experimental work has shown that

cylindrical vessels will buckle at values well below that given by Equation 14.29. For steels at ambient temperature $E_Y = 200{,}000\ \text{N/mm}^2$ and Equation 14.30 with a factor of safety of 12 gives:

$$\sigma_c = 2 \times 10^4 \left(\frac{t}{D_o}\right) \quad \text{N/mm}^2 \tag{14.31}$$

The maximum compressive stress in a vessel wall should not exceed that given by Equation 14.31 or the maximum allowable design stress for the material, whichever is the least. For detailed design, the ASME BPV Code Sec. VIII should be consulted and the recommended procedure in the code should be followed.

Stiffening

As with vessels under external pressure, the resistance to failure by buckling can be increased significantly by the use of stiffening rings or longitudinal strips. Methods for estimating the critical buckling stress for stiffened vessels are given in the standards and codes.

Loading

The loads to which a vessel may be subjected will not all occur at the same time. For example, it is the usual practice to assume that the maximum wind load will not occur simultaneously with a major earthquake.

The vessel must be designed to withstand the worst combination of the loads likely to occur in the following situations:

1. During erection (or dismantling) of the vessel.
2. With the vessel erected but not operating.
3. During testing (the hydraulic pressure test).
4. During normal operation.

14.8.1 Weight loads

The major sources of dead weight loads are:

1. The vessel shell.
2. The vessel fittings: manways, nozzles.
3. Internal fittings: plates (plus the fluid on the plates); heating and cooling coils.
4. External fittings: ladders, platforms, piping.
5. Auxiliary equipment that is not self-supported; condensers, agitators.
6. Insulation.
7. The weight of liquid to fill the vessel. The vessel will be filled with water for the hydraulic pressure test and may fill with process liquid due to misoperation.

Note: For vessels on a skirt support (see Section 14.9.2), the weight of the liquid to fill the vessel will be transferred directly to the skirt.

The weight of the vessel and fittings can be calculated from the preliminary design sketches. The weights of standard vessel components: heads, shell plates, manways, branches and nozzles, are given in various handbooks: Megyesy (2008) and Brownell and Young (1959).

For preliminary calculations, the approximate weight of a cylindrical vessel with domed ends, and uniform wall thickness, can be estimated from the following equation:

$$W_v = C_w\, \pi\, \rho_m\, D_m\, g(H_v + 0.8D_m)\, t \times 10^{-3} \tag{14.32}$$

where

W_v = total weight of the shell, excluding internal fittings, such as plates, N,
C_w = a factor to account for the weight of nozzles, manways, internal supports, etc., which can be taken as
= 1.08 for vessels with only a few internal fittings,
= 1.15 for distillation columns, or similar vessels, with several manways, and with plate support rings or equivalent fittings,

H_v = height, or length, between tangent lines (the length of the cylindrical section), m,
g = gravitational acceleration, 9.81 m/s^2
t = wall thickness, mm,
ρ_m = density of vessel material, kg/m^3 (see Table 6.2),
D_m = mean diameter of vessel = $(D_i + t \times 10^{-3})$, m.

For a steel vessel, Equation 14.32 reduces to:

$$W_v = 240\, C_w D_m\, (H_v + 0.8 D_m)\, t \tag{14.33}$$

The following values can be used as a rough guide to the weight of fittings; see Nelson (1963):

1. Caged ladders, steel, 360 N/m length,
2. Plain ladders, steel, 150 N/m length,
3. Platforms, steel, for vertical columns, 1.7 kN/m^2 area,
4. Contacting plates, steel, including typical liquid loading, 1.2 kN/m^2 plate area.

Typical values for the density of insulating materials are (all kg/m^3):

Foam glass	150
Mineral wool	130
Fiberglass	100
Calcium silicate	200

These densities should be doubled to allow for attachment fittings, sealing, and moisture absorption.

14.8.2 Wind loads (tall vessels)

Wind loading will only be important on tall columns installed in the open. Columns and chimney stacks are usually free standing, mounted on skirt supports, and not attached to structural steel work. Under these conditions the vessel under wind loading acts as a cantilever beam (Fig. 14.11). For a uniformly loaded cantilever, the bending moment at any plane is given by:

$$M_x = \frac{W x^2}{2} \tag{14.34}$$

where x is the distance measured from the free end and W the load per unit length (Newtons per meter run).

So the bending moment, and hence the bending stress, will vary parabolically from zero at the top of the column to a maximum value at the base. For tall columns, the bending stress due to wind loading will often be greater than direct stress due to pressure and will determine the plate thickness required. The most economical design will be one in which the plate thickness is progressively increased from the top to the base of the column, with the thickness at the top being sufficient for the pressure load and that at the base sufficient for the pressure plus the maximum bending moment.

Any local increase in the column area presented to the wind will give rise to a local, concentrated load (Fig. 14.12). The bending moment at the column base caused by a concentrated load is given by:

$$M_p = F_p H_p \tag{14.35}$$

where F_p = local, concentrated load,
H_p = the height of the concentrated load above the column base.

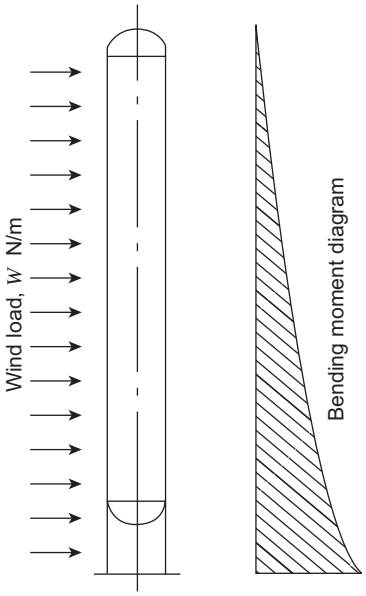


FIG. 14.11 Wind loading on a tall column.

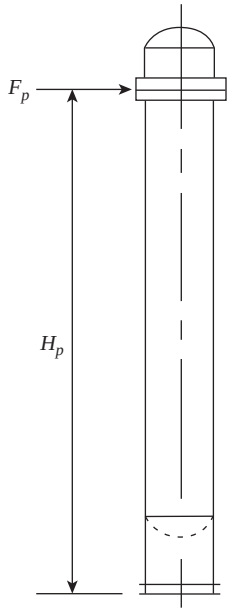


FIG. 14.12 Local wind loading.

Dynamic wind pressure

The load imposed on any structure by the action of the wind will depend on the shape of the structure and the wind velocity.

$$P_w = \frac{1}{2} C_d \rho_a u_w^2 \tag{14.36}$$

where P_w = wind pressure (load per unit area),
C_d = drag coefficient (shape factor),
ρ_a = density of air,
u_w = wind velocity.

The drag coefficient is a function of the shape of the structure and the wind velocity (Reynolds number).

For a smooth cylindrical column or stack, the following semi-empirical equation can be used to estimate the wind pressure:

$$P_w = 0.05 u_w^2 \tag{14.37}$$

where P_w = wind pressure, N/m^2
u_w = wind speed, km/h

If the column outline is broken up by attachments, such as ladders or pipe work, the factor of 0.05 in Equation 14.37 should be increased to 0.07 to allow for the increased drag.

A column must be designed to withstand the highest wind speed that is likely to be encountered at the site during the life of the plant. The probability of a given wind speed occurring can be predicted by studying meteorological records for the site location. Data and design methods for wind loading are given in the Engineering Sciences Data Unit (ESDU) Wind Engineering Series (www.esdu.com). Design loadings for locations in the United States are given by Moss and Basic (2013), Megyesy (2008), and Escoe (1994). A wind speed of 160 km/h (100 mph) can be used for preliminary design studies, equivalent to a wind pressure of 1280 N/m^2 (25 lb/ft^2).

At any site, the wind velocity near the ground will be lower than that higher up (due to the boundary layer), and in some design methods a lower wind pressure is used at heights below about 20 m, typically taken as one-half of the pressure above this height.

The loading per unit length of the column can be obtained from the wind pressure by multiplying by the effective column diameter: the outside diameter plus an allowance for the thermal insulation and attachments such as pipes and ladders.

$$W = P_w \, D\text{eff} \tag{14.38}$$

An allowance of 0.4 m should be added for a caged ladder. The calculation of the wind load on a tall column, and the induced bending stresses, is illustrated in Example 14.2. Further examples of the design of tall columns are given by Brownell (1963), Henry (1973), Bednar (1990), Escoe (1994), and Jawad and Farr (2018).

Deflection of tall columns

Tall columns sway in the wind. The allowable deflection will normally be specified as less than 150 mm per 30 m of height (6 in per 100 ft).

For a column with a uniform cross-section, the deflection can be calculated using the formula for the deflection of a uniformly loaded cantilever. A method for calculating the deflection of a column where the wall thickness is not constant is given by Tang (1968).

Wind-induced vibrations

Vortex shedding from tall thin columns and stacks can induce vibrations which, if the frequency of shedding of eddies matches the natural frequency of the column, can be severe enough to cause premature failure of the vessel by fatigue. The effect of vortex shedding should be investigated for free-standing columns with height-to-diameter ratios greater than 10. Methods for estimating the natural frequency of columns are given by Freese (1959) and DeGhetto and Long (1966).

Helical strakes (strips) are fitted to the tops of tall, smooth chimneys to change the pattern of vortex shedding and so prevent resonant oscillation. The same effect will be achieved on a tall column by distributing any attachments (ladders, pipes, and platforms) around the column.

14.8.3 Earthquake loading

The movement of the earth's surface during an earthquake produces horizontal shear forces on tall, self-supported vessels, the magnitude of which increases from the base upward. The total shear force on the vessel will be given by:

$$F_s = a_e \left(\frac{W_v}{g} \right) \tag{14.39}$$

where a_e = the acceleration of the vessel due to the earthquake,
g = the acceleration due to gravity,
W_v = total weight of the vessel and contents.

The term (a_e/g) is called the seismic constant C_e, and is a function of the natural period of vibration of the vessel and the severity of the earthquake. Values of the seismic constant have been determined empirically from studies of the damage caused by earthquakes and are available for those geographical locations that are subject to earthquake activity. Values for sites in the United States and procedures for determining the stresses induced in tall columns are given by Megyesy (2008), Escoe (1994), and Moss and Basic (2013).

14.8.4 Eccentric loads (tall vessels)

Ancillary equipment attached to a tall vessel will subject the vessel to a bending moment if the center of gravity of the equipment does not coincide with the center line of the vessel (Fig. 14.13). The moment produced by small fittings, such as ladders, pipes, and manways, will be small and can be neglected. That produced by heavy equipment, such as reflux condensers and side platforms, can be significant and should be considered. The moment is given by:

$$M_e = W_e L_o \tag{14.40}$$

where W_e = dead weight of the equipment,
L_o = distance between the center of gravity of the equipment and the column center line.

To avoid putting undue stress on the column walls, equipment (such as reflux condensers and overhead receiving drums) is usually not attached to the top of a column, but is instead located adjacent to the column in the plant structure. Condensers and receiving vessels are often placed above grade level to provide net positive suction head for reflux and overhead pumps sited at grade.

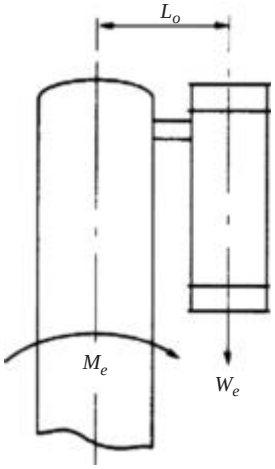


FIG. 14.13 Bending moment due to offset equipment.

14.8.5 Torque

Any horizontal force imposed on the vessel by ancillary equipment, the line of thrust of which does not pass through the center line of the vessel, will produce a torque on the vessel. Such loads can arise through wind pressure on piping and other attachments; however, the torque will normally be small and usually can be disregarded. The pipe work and the connections for any ancillary equipment will be designed so as not to impose a significant load on the vessel.

Example 14.2

Make a preliminary estimate of the plate thickness required for the distillation column specified here:

Height, between tangent lines	50 m
Diameter	2 m
Hemispherical head	
Skirt support, height	3 m
100 sieve plates, equally spaced	
Insulation, mineral wool	75 mm thick
Material of construction, stainless steel, maximum allowable stress	135 N/mm^2 at design temperature 200 °C
Operating pressure	10 bar (absolute)
Vessel to be fully radiographed (joint efficiency 1)	
Process service	Gasoline debutanizer

Solution

Design pressure; take as 10% above operating pressure:

$$= (10 - 1) \times 1.1 = 9.9 \text{ bar, say } 10 \text{ bar}$$
$$= 1.0 \text{ N/mm}^2$$

Minimum thickness required for pressure loading:

$$t = \frac{1 \times 2 \times 10^3}{(2 \times 135 \times 1) - (1.2 \times 1)} = 7.4 \text{ mm} \quad (14.13)$$

A much thicker wall will be needed at the column base to withstand the wind and dead weight loads.

As a first trial, divide the column into five sections (courses), with the thickness increasing by 2 mm per section. Try 10, 12, 14, 16, 18 mm.

Dead weight of vessel

Though Equation 14.33 only applies strictly to vessels with uniform thickness, it can be used to get a rough estimate of the weight of this vessel by using the average thickness in the equation, 14 mm.

Take $C_w = 1.15$, vessel with plates

$$D_m = 2 + 14 \times 10^{-3} = 2.014 \text{ m}$$
$$H_v = 50 \text{ m}$$
$$t = 14 \text{ mm}$$
$$W_v = 240 \times 1.15 \times 2.014(50 + 0.8 \times 2.014)14 \quad (14.33)$$
$$= 401,643 \text{ N}$$
$$= 402 \text{ kN}$$

Weight of plates:

plate area $= \pi/4 \times 2^2 = 3.14 \text{ m}^2$
weight of a plate including liquid on it (see Section 14.8.1) $\approx 1.2 \times 3.14 = 3.8$ kN
100 plates $= 100 \times 3.8 = 380$ kN

Weight of insulation:

mineral wool density = 130 kg/m^3
approximate volume of insulation = $\pi \times 2 \times 50 \times 75 \times 10^{-3}$
= 23.6 m^3
weight = $23.6 \times 130 \times 9.81 = 30{,}049$ N
double this to allow for fittings, etc. = 60 kN
Total weight:

Shell	402
plates & contents	380
Insulation	60
	842 kN

Note that the weight of the contents of the column would be substantially greater if the column were flooded or entirely filled with liquid. This is the case during hydraulic testing, which should be examined as a different loading scenario.

Wind loading

Take dynamic wind pressure as 1280 N/m^2, corresponding to 160 kph (100 mph).

$$\text{Mean diameter, including insulation} = 2 + 2(14 + 75) \times 10^{-3} = 2.18 \text{ m}$$

$$\text{Loading (per linear meter) } W = 1280 \times 2.18 = 2790 \text{ N/m} \tag{14.38}$$

Bending moment at bottom tangent line:

$$M_x = \frac{2790}{2} \times 50^2 = 3{,}487{,}500 \text{ Nm} \tag{14.34}$$

Analysis of stresses

At bottom tangent line:
Pressure stresses:

$$\sigma_L = \frac{1.0 \times 2 \times 10^3}{4 \times 18} = 27.8 \text{ N/mm}^2 \tag{14.7}$$

$$\sigma_h = \frac{1 \times 2 \times 10^3}{2 \times 18} = 55.6 \text{ N/mm}^2 \tag{14.10}$$

Dead weight stress:

$$\sigma_w = \frac{W_v}{\pi(D_i + t)t} = \frac{842 \times 10^3}{\pi(200 + 18)18} = 7.4 \text{ N/mm}^2 \text{(compressive)} \tag{14.22}$$

Bending stresses:

$$D_o = 2000 + 2 \times 18 = 2036 \text{ mm}$$

$$I_v = \frac{\pi}{64}\left(2036^4 - 2000^4\right) = 5.81 \times 10^{10} \text{ mm}^4 \tag{14.24}$$

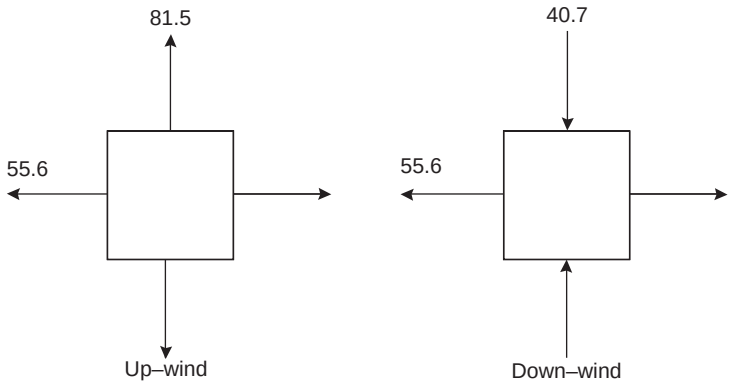
$$\sigma_b = \pm \frac{3{,}487{,}500 \times 10^3}{5.81 \times 10^{10}} \left(\frac{2000}{2} + 18 \right) = \pm 61.11 \text{ N/mm}^2 \tag{14.23}$$

The resultant longitudinal stress is:

$$\sigma_z = \sigma_L + \sigma_w \pm \sigma_b$$

σ_w is compressive and therefore negative.
σ_z (upwind) $= 27.8 - 7.4 + 61.1 = +81.5$ N/mm^2.
σ_z (downwind) $= 27.8 - 7.4 - 61.1 = -40.7$ N/mm^2.

As there is no torsional shear stress, the principal stresses will be σ_z and σ_h. The radial stress is negligible: $(P_i/2) = 0.5$ N/mm^2.



The greatest difference between the principal stresses will be on the downwind side:

$$(55.6 - (-40.7)) = \underline{\underline{95.5 \text{ N/mm}^2}}$$

well below the maximum allowable design stress.

Note that the bending stress due to wind loading is much larger than the dead weight stress. The hydraulic testing case will have a greater dead weight when the vessel is filled with water, but a simple calculation shows that the maximum weight of water in the vessel (neglecting volume of vessel internals) is $\pi/12 \times \rho \times g\ (3D_i^2 L + 2D_i^3) = 1582$ kN. If this is added to the total weight calculated earlier, then the dead weight stress will increase by about a factor 3. This is still a lot less than the bending stress due to wind load, so the wind load case is the governing case. The hydraulic test will obviously not be scheduled for a day on which 100-mph winds may occur.

Check elastic stability (buckling)

Critical buckling stress:

$$\sigma_c = 2 \times 10^4 \left(\frac{18}{2036} \right) = \underline{\underline{176.8 \text{ N/mm}^2}} \tag{14.31}$$

The maximum compressive stress will occur when the vessel is not under pressure $= 7.4 + 61.1 = 68.5$, well below the critical buckling stress.

So the design is satisfactory. The designer could reduce the plate thickness and recalculate.

14.9 Vessel supports

The method used to support a vessel will depend on the size, shape, and weight of the vessel; the design temperature and pressure; the vessel location and arrangement; and the internal and external fittings and attachments. Horizontal vessels are usually mounted on two saddle supports (Fig. 14.14). Skirt supports are used for tall, vertical columns (Fig. 14.15). Brackets, or lugs, are used for all types of vessels (Fig. 14.16). The supports must be designed to

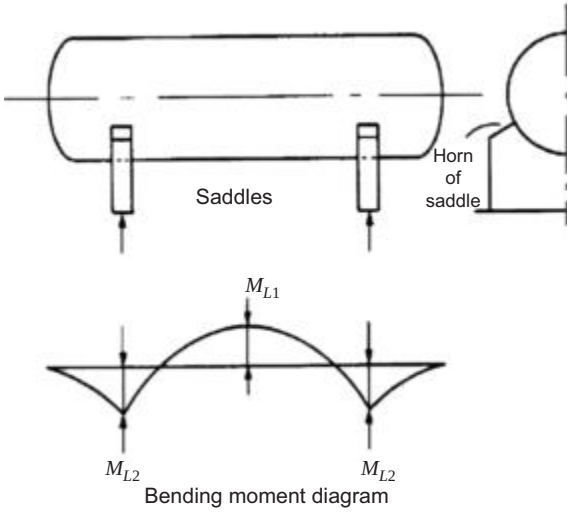


FIG. 14.14 Horizontal cylindrical vessel on saddle supports.

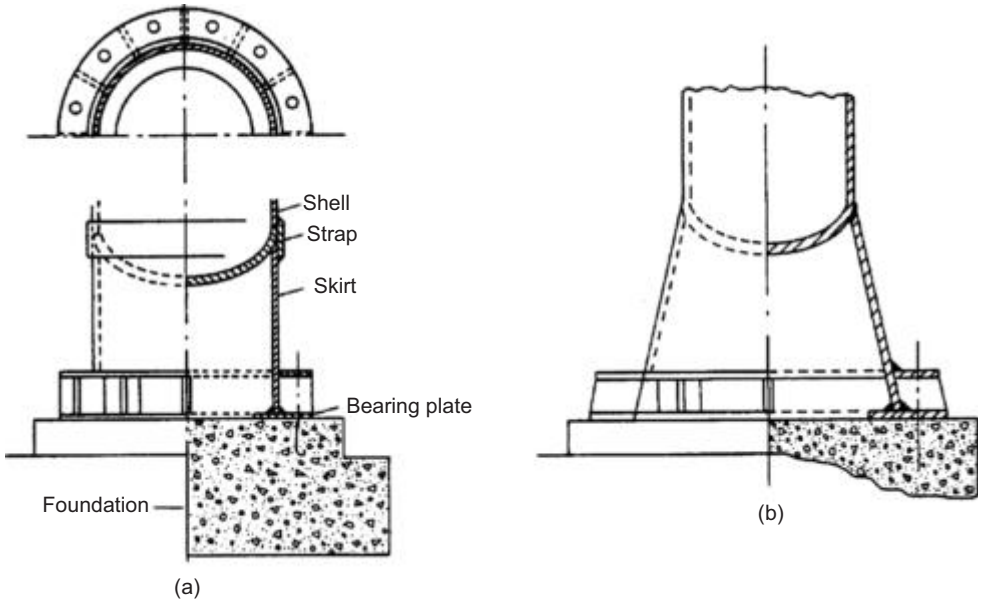


FIG. 14.15 Typical skirt-support designs. (a) Straight skirt. (b) Conical skirt.

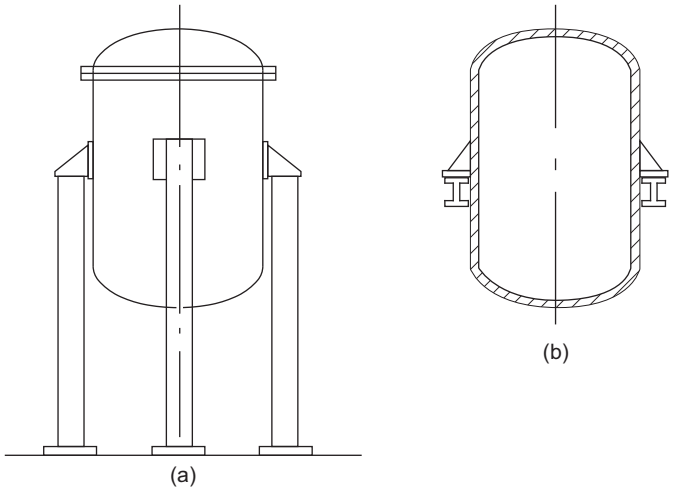


FIG. 14.16 Bracket supports. (a) Supported on legs. (b) Supported from steel work.

carry the weight of the vessel and contents and any superimposed loads, such as wind loads. Supports will impose localized loads on the vessel wall, and the design must be checked to ensure that the resulting stress concentrations are below the maximum allowable design stress. Supports should be designed to allow easy access to the vessel and fittings for inspection and maintenance.

14.9.1 Saddle supports

Though saddles are the most commonly used support for horizontal cylindrical vessels, legs can be used for small vessels. A horizontal vessel will normally be supported at two cross-sections; if more than two saddles are used, the distribution of the loading is uncertain.

A vessel supported on two saddles can be considered a simply supported beam, with an essentially uniform load, and the distribution of longitudinal axial bending moment will be as shown in Fig. 14.14. Maxima occur at the supports and at mid-span. The theoretical optimum position of the supports to give the least maximum bending moment will be the position at which the maxima at the supports and at mid-span are equal in magnitude. For a uniformly loaded beam, the position will be at 21% of the span in from each end. The saddle supports for a vessel will usually be located nearer the ends than this value to make use of the stiffening effect of the ends.

In addition to the longitudinal bending stress, a vessel supported on saddles will be subjected to tangential shear stresses, which transfer the load from the unsupported sections of the vessel to the supports and to circumferential bending stresses. All these stresses need to be considered in the design of large, thin-walled, vessels to ensure that the resultant stress does not exceed the maximum allowable design stress or the critical buckling stress for the material. A detailed stress analysis is beyond the scope of this book. A complete analysis of the stress induced in the shell by the supports is given by Zick (1951). Zick's method forms the basis of the design methods given in the national codes and standards. The method is also given by Brownell and Young (1959), Escoe (1994), and Megyesy (2008).

Design of saddles

The saddles must be designed to withstand the load imposed by the weight of the vessel and contents. They are constructed of bricks or concrete or are fabricated from steel plate. The contact angle should not be less than 120 degrees, and will not normally be greater than 150 degrees. Wear plates are often welded to the shell wall to reinforce the wall over the area of contact with the saddle.

The dimensions of typical "standard" saddle designs are given in Fig. 14.17. To take up any thermal expansion of the vessel, such as that in heat exchangers, the anchor bolt holes in one saddle can be slotted.

Procedures for the design of saddle supports are given by Brownell and Young (1959), Megyesy (2008), Escoe (1994), and Moss and Basic (2013).

14.9.2 Skirt supports

A skirt support consists of a cylindrical or conical shell welded to the base of the vessel. A flange at the bottom of the skirt transmits the load to the foundations. Typical designs are shown in Fig. 14.15. Openings must be provided in the skirt for access and for any connecting pipes; the openings are normally reinforced. The skirt may be welded to the bottom head of the vessel (Fig. 14.18a) or welded flush with the shell (Fig. 14.18b) or welded to the outside of the vessel shell (Fig. 14.18c). The arrangement shown in Fig. 14.18(b) is usually preferred.

Skirt supports are recommended for vertical vessels, as they do not impose concentrated loads on the vessel shell; they are particularly suitable for use with tall columns subject to wind loading, as the support is equally strong in all directions.

Skirt thickness

The skirt thickness must be sufficient to withstand the dead-weight loads and bending moments imposed on it by the vessel; it will not be under the vessel pressure.

The resultant stresses in the skirt will be:

$$\sigma_s \text{ (tensile)} = \sigma_{bs} - \sigma_{ws} \tag{14.41}$$

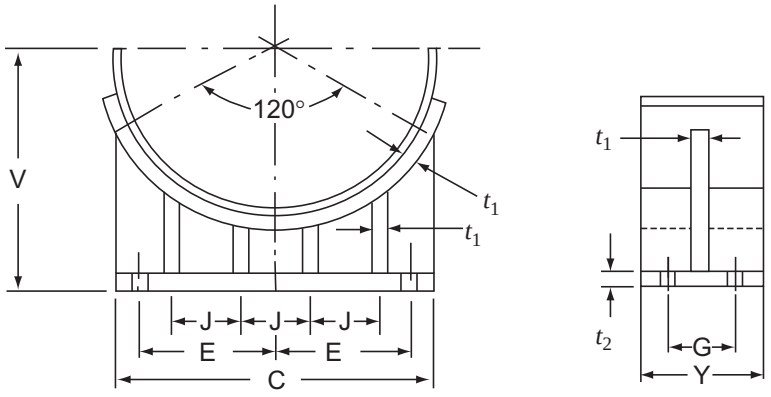
and

$$\sigma_s \text{ (compressive)} = \sigma_{bs} + \sigma_{ws} \tag{14.42}$$

where

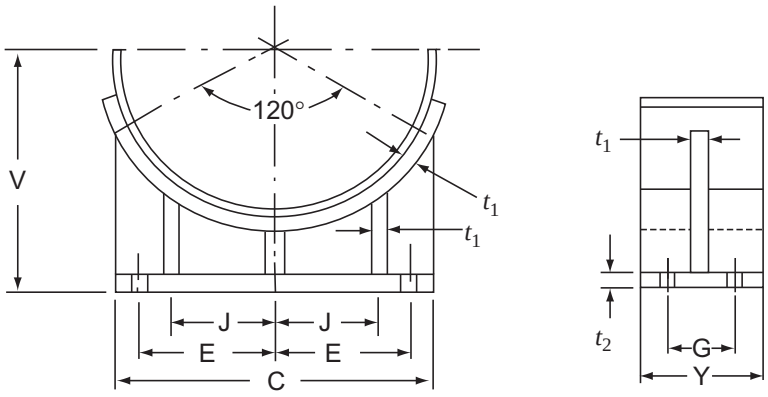
σ_{bs} = bending stress in the skirt

$$= \frac{4\,M_s}{\pi(D_s + t_{sk})\,t_{sk}D_s}, \tag{14.43}$$



Vessel Diam. (m)	Maximum Weight (kN)	Dimensions (m)						mm			
		V	*Y*	*C*	*E*	*J*	*G*	t_2	t_1	Bolt Diam.	Bolt Holes
0.6	35	0.48	0.15	0.55	0.24	0.190	0.095	6	5	20	25
0.8	50	0.58	0.15	0.70	0.29	0.225	0.095	8	5	20	25
0.9	65	0.63	0.15	0.81	0.34	0.275	0.095	10	6	20	25
1.0	90	0.68	0.15	0.91	0.39	0.310	0.095	11	8	20	25
1.2	180	0.78	0.20	1.09	0.45	0.360	0.140	12	10	24	30

(a) All contacting edges fillet welded



Vessel Diam. (m)	Maximum Weight (kN)	Dimensions (m)						mm			
		V	*Y*	*C*	*E*	*J*	*G*	t_2	t_1	Bolt Diam.	Bolt Holes
1.4	230	0.88	0.20	1.24	0.53	0.305	0.140	12	10	24	30
1.6	330	0.98	0.20	1.41	0.62	0.350	0.140	12	10	24	30
1.8	380	1.08	0.20	1.59	0.71	0.405	0.140	12	10	24	30
2.0	460	1.18	0.20	1.77	0.80	0.450	0.140	12	10	24	30
2.2	750	1.28	0.225	1.95	0.89	0.520	0.150	16	12	24	30
2.4	900	1.38	0.225	2.13	0.98	0.565	0.150	16	12	27	33
2.6	1000	1.48	0.225	2.30	1.03	0.590	0.150	16	12	27	33
2.8	1350	1.58	0.25	2.50	1.10	0.625	0.150	16	12	27	33
3.0	1750	1.68	0.25	2.64	1.18	0.665	0.150	16	12	27	33
3.2	2000	1.78	0.25	2.82	1.26	0.730	0.150	16	12	27	33
3.6	2500	1.98	0.25	3.20	1.40	0.815	0.150	16	12	27	33

(b) All contacting edges fillet welded.

FIG. 14.17 Standard steel saddles. (a) For vessels up to 1.2 m. (b) For vessels greater than 1.2 m. *Adapted from Bhattacharyya 2011.*

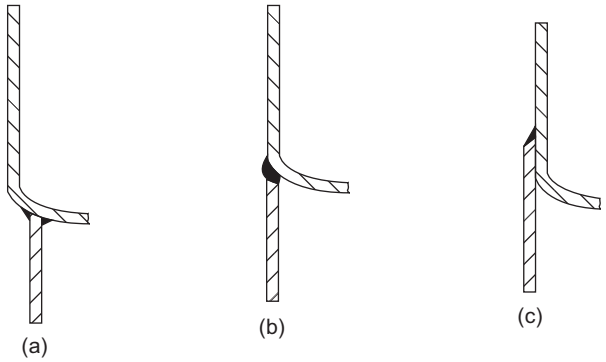


FIG. 14.18 Skirt-support welds.

σ_{ws} = the dead weight stress in the skirt,

$$= \frac{W_v}{\pi(D_s + t_{sk})\, t_{sk}} \tag{14.44}$$

where

M_s = maximum bending moment, evaluated at the base of the skirt (due to wind, seismic, and eccentric loads; see Section 14.8),
W_v = total weight of the vessel and contents (see Section 14.8),
D_s = inside diameter of the skirt, at the base,
t_{sk} = skirt thickness.

The skirt thickness should be such that under the worst combination of wind and dead-weight loading, the following design criteria are not exceeded:

$$\sigma_s \text{ (tensile)} < S_s E \sin\theta_s \tag{14.45}$$

$$\sigma_s \text{ (compressive)} < 0.125\, E_Y \left(\frac{t_{sk}}{D_s}\right) \sin\theta_s \tag{14.46}$$

where

S_s = maximum allowable design stress for the skirt material, normally taken at ambient temperature, 20 °C,
E = weld joint efficiency, if applicable,
θ_s = base angle of a conical skirt, normally 80 to 90 degrees.

The minimum thickness should be not less than 6 mm.

Where the vessel wall will be at a significantly higher temperature than the skirt, discontinuity stresses will be set up due to differences in thermal expansion. Methods for calculating the thermal stresses in skirt supports are given by Weil and Murphy (1960) and Bergman (1963).

Base ring and anchor bolt design

The loads carried by the skirt are transmitted to the foundation slab by the skirt base ring (bearing plate). The moment produced by wind and other lateral loads will tend to overturn the vessel; this will be opposed by the couple set up by the weight of the vessel and the tensile load in the anchor bolts. Various base ring designs are used with skirt supports. The simplest types, suitable for small vessels, are the rolled angle and plain flange rings shown in Fig. 14.19 (a) and (b). For larger columns, a double ring stiffened by gussets (Fig. 14.19c) or chair supports are used. Design methods for base rings, and methods for sizing the anchor bolts, are given by Brownell and Young (1959). For preliminary design, the shortcut method and nomographs given by Scheiman (1963) can be used. Scheiman's method is based on a more detailed procedure for the design of base rings and foundations for columns and stacks given by Marshall (1958).

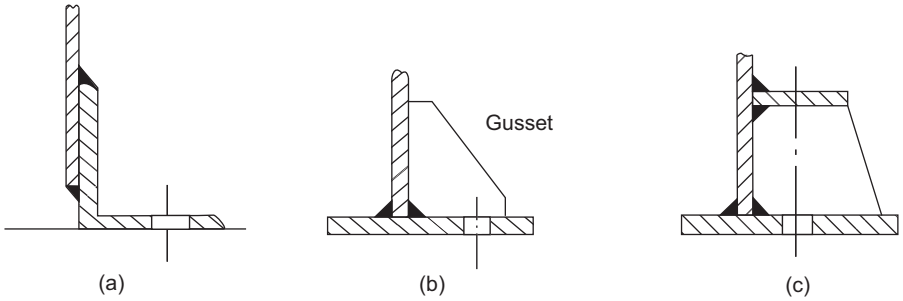


FIG. 14.19 Flange ring designs. (a) Rolled angle. (b) Single plate with gusset. (c) Double plate with gusset.

Example 14.3

Design a skirt support for the column specified in Example 14.2.

Solution

Try a straight cylindrical skirt ($\theta_s = 90°$) of plain carbon steel, maximum allowable stress 89 N/mm^2, and Young's modulus 200,000 N/mm2 at ambient temperature.

The maximum dead weight load on the skirt will occur when the vessel is full of water.

$$\text{Approximate weight} = \left(\frac{\pi}{4} \times 2^2 \times 50\right) 1000 \times 9.81$$

$$= 1{,}540{,}951 \text{ N}$$

$$= 1541 \text{ kN}$$

$$\text{Weight of vessel from Example 14.2} = 842 \text{ kN}$$

$$\text{Total weight} = 1541 + 842 = 2383 \text{ kN}$$

$$\text{Wind loading, from Example 14.2} = 2.79 \text{ kN/m}$$

$$\text{Bending moment at base of skirt} = 2.79 \times \frac{53^2}{2}$$

$$= 3919 \text{ kNm} \tag{14.34}$$

As a first trial, take the skirt thickness as the same as that of the bottom section of the vessel, 18 mm.

$$\sigma_{bs} = \frac{4 \times 3919 \times 10^3 \times 10^3}{\pi(2000 + 18)\, 2000 \times 18} \tag{14.43}$$

$$= 68.7 \text{ N/mm}^2$$

$$\sigma_{ws} \text{ (test)} = \frac{2383 \times 10^3}{\pi(2000 + 18)\, 18} = 20.9 \text{ N/mm}^2 \tag{14.43}$$

$$\sigma_{ws} \text{ (operating)} = \frac{842 \times 10^3}{\pi(2000 + 18)\, 18} = 7.4 \text{ N/mm}^2 \tag{14.44}$$

Note: the "test" condition is with the vessel full of water for the hydraulic test. In estimating total weight, the weight of liquid on the plates has been counted twice. The weight has not been adjusted to allow for this, as the error is small and on the "safe side."

$$\text{Maximum } \hat{\sigma}_s \text{ (compressive)} = 68.7 + 20.9 = 89.6 \text{ N/mm}^2 \tag{14.42}$$

$$\text{Maximum } \hat{\sigma}_s \text{ (tensile)} = 68.7 - 7.4 = 61.3 \text{ N/mm}^2 \tag{14.41}$$

Take the joint efficiency E as 0.85.
Criteria for design:

$$\widehat{\sigma}_s \text{ (tensile)} < S_s E \sin\theta \tag{14.45}$$

$$61.3 < 0.85 \times 89 \sin 90$$
$$61.3 < 75.6$$

$$\widehat{\sigma}_s \text{ (compressive)} < 0.125 E_Y \left(\frac{t_{sk}}{D_s}\right) \sin\theta$$

$$89.6 < 0.125 \times 200,000 \left(\frac{18}{2000}\right) \sin 90 \tag{14.46}$$

$$89.6 < 225$$

Both criteria are satisfied; add 2 mm for corrosion gives a design thickness of 20 mm.

14.9.3 Bracket supports

Brackets, or lugs, can be used to support vertical vessels. The bracket may rest on the building structural steel work, or the vessel may be supported on legs (see Fig. 14.16).

The main load carried by the brackets will be the weight of the vessel and contents; in addition, the bracket must be designed to resist the load due to any bending moment due to wind or other loads. If the bending moment is likely to be significant, skirt supports should be considered in preference to bracket supports.

As the reaction on the bracket is eccentric (Fig. 14.20), the bracket will impose a bending moment on the vessel wall. The point of support, at which the reaction acts, should be made as close to the vessel wall as possible, allowing for the thickness of any insulation. Methods for estimating the magnitude of the stresses induced in the vessel wall by bracket supports are given by Brownell and Young (1959) and by Wolosewick (1951). Backing plates or collars are often used to carry the bending loads.

The brackets and supporting steel work can be designed using the usual methods for structural steelwork. Suitable methods are given by Bednar (1986) and Moss and Basic (2013). A quick method for sizing vessel reinforcing rings (backing plates) for bracket supports is given by Mahajan (1977).

Typical bracket designs are shown in Fig. 14.21(a) and (b). The loads that steel brackets with these proportions will support are given by the following formula:

Single-gusset plate design (see Fig. 14.21a):

$$F_{bs} = 60 L_d t_c \tag{14.47}$$

Double-gusset plate design (see Fig. 14.21b):

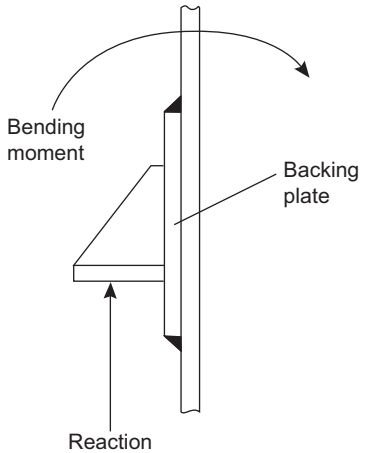


FIG. 14.20 Loads on a bracket support.

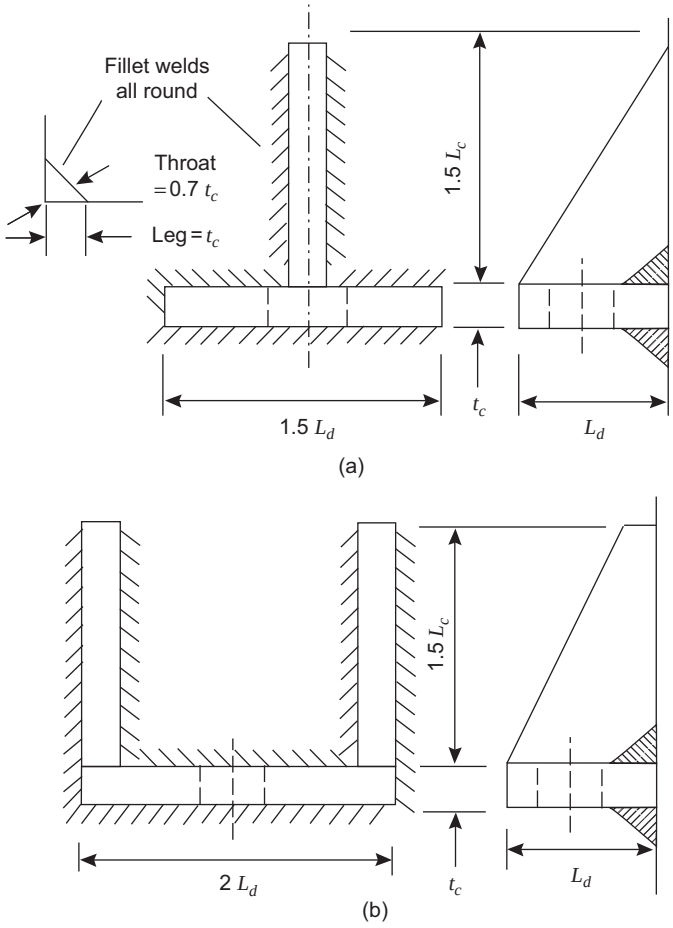


FIG. 14.21 Bracket designs. (a) Single gusset plate. (b) Double gusset plate.

$$F_{bs} = 120 L_d \, t_c \tag{14.48}$$

where F_{bs} = maximum design load per bracket, N
L_d = the characteristic dimension of bracket (depth), mm
t_c = thickness of plate, mm

14.10 Bolted flanged joints

Flanged joints are used for connecting pipes and instruments to vessels, for manhole covers, and for removable vessel heads when ease of access is required. Flanges may also be used on the vessel body when it is necessary to divide the vessel into sections for transport or maintenance. Flanged joints are also used to connect pipes to other equipment, such as pumps and valves. Screwed joints are often used for small-diameter pipe connections, below 2 in (50 mm). Flanged joints are also used for connecting pipe sections where ease of assembly and dismantling is required for maintenance, but pipework will normally be welded to reduce costs.

Flanges range in size from a few millimeters in diameter for small pipes to several meters diameter for those used as body or head flanges on vessels.

14.10.1 Types of flanges and selection

Several different types of flanges are used for various applications. The principal types used in the process industries are:

1. Welding-neck flanges
2. Slip-on flanges, hub and plate types
3. Lap-joint flanges
4. Screwed flanges
5. Blank, or blind, flanges

Welding-neck flanges (Fig. 14.22a) have a long tapered hub between the flange ring and the welded joint. This gradual transition of the section reduces the discontinuity stresses between the flange and branch and increases the strength of the flange assembly. Welding-neck flanges are suitable for extreme service conditions, where the flange is likely to be subjected to temperature, shear, and vibration loads. They will normally be specified for the connections and nozzles on process vessels and process equipment.

Slip-on flanges (Fig. 14.22b) slip over the pipe or nozzle and are welded externally and usually also internally. The end of the pipe is set back from 0 to 2.0 mm. The strength of a slip-on flange is from one-third to two-thirds that of the corresponding standard welding-neck flange. Slip-on flanges are cheaper than welding-neck flanges and are easier to align but have poor resistance to shock and vibration loads. Slip-on flanges are generally used for pipe work. Fig. 14.22(b) shows a forged flange with a hub; for light duties, slip-on flanges can be cut from plate.

Lap-joint flanges (Fig. 14.22c) are used for pipework. They are economical when used with expensive alloy pipe, such as stainless steel, as the flange can be made from inexpensive carbon steel. Usually a short-lapped nozzle is welded to the pipe, but with some schedules of pipe, the lap can be formed on the pipe itself; this will give a cheap method of pipe assembly. Lap-joint flanges are sometimes known as "Van-stone flanges."

Screwed flanges (Fig. 14.22d) are used to connect screwed fittings to flanges. They are also sometimes used for alloy pipe that is difficult to weld satisfactorily.

Blind flanges (blank flanges) are flat plates used to blank off flange connections and as covers for manholes and inspection ports.

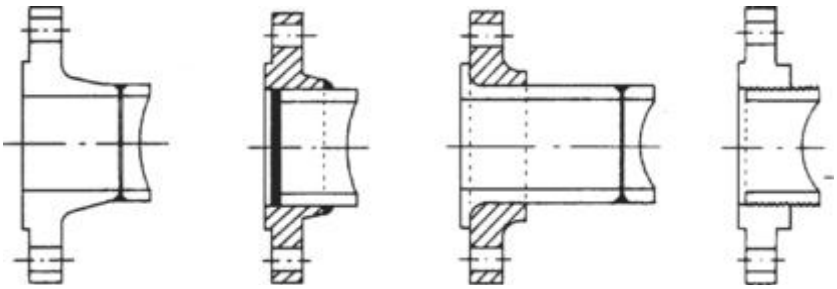


FIG. 14.22 Flange types. (a) Welding neck. (b) Slip-on. (c) Lap joint. (d) Screwed.

14.10.2 Gaskets

Gaskets are used to make a leak-tight joint between two surfaces. It is impractical to machine flanges to the degree of surface finish that would be required to make a satisfactory seal under pressure without a gasket. Gaskets are made from "semi-plastic" materials that will deform and flow under load to fill the surface irregularities between the flange faces yet retain sufficient elasticity to take up the changes in the flange alignment that occur under load.

A great variety of proprietary gasket materials is used, and reference should be made to the manufacturers' catalogues and technical manuals when selecting gaskets for a particular application. Design data for some of the more commonly used gasket materials are given in Table 14.4. Further data can be found in the ASME BPV Code Sec. VIII D.1 Mandatory Appendix 2, ASME B16.20 and in Green and Southard (2018). The minimum seating stress y is the force per unit area (pressure) on the gasket that is required to cause the material to flow and fill the surface irregularities in the gasket face.

The gasket factor m is the ratio of the gasket stress (pressure) under the operating conditions to the internal pressure in the vessel or pipe. The internal pressure will force the flanges' faces apart, so the pressure on the gasket under operating conditions will be lower than the initial tightening-up pressure. The gasket factor gives the minimum pressure that must be maintained on the gasket to ensure a satisfactory seal.

The following factors must be considered when selecting a gasket material:

1. The process conditions: pressure, temperature, corrosive nature of the process fluid
2. Whether repeated assembly and disassembly of the joint are required
3. The type of flange and flange face (see Section 14.10.3)

Up to pressures of 20 bar, the operating temperature and corrosiveness of the process fluid will be the controlling factor in gasket selection. Vegetable fiber and synthetic rubber gaskets can be used at temperatures of up to 100 °C. Solid polyfluorocarbon (Teflon) and compressed asbestos gaskets can be used to a maximum temperature of about 260°C. Metal-reinforced gaskets can be used up to around 450 °C. Plain soft metal gaskets are normally used for higher temperatures.

14.10.3 Flange faces

Flanges are also classified according to the type of flange face used. There are two basic types:

1. Full-faced flanges (Fig. 14.23a), where the face contact area extends outside the circle of bolts over the full face of the flange.
2. Narrow-faced flanges (Fig. 14.23b, c, and d), where the face contact area is located within the circle of bolts.

Full face, wide-faced flanges are simple and inexpensive, but are only suitable for low pressures. The gasket area is large, and an excessively high bolt tension would be needed to achieve sufficient gasket pressure to maintain a good seal at high operating pressures.

The raised-face, narrow-faced flange shown in Fig. 14.23(b) is probably the most commonly used type of flange for process equipment.

Where the flange has a plain face, as in Fig. 14.23(b), the gasket is held in place by friction between the gasket and flange surface. In the spigot and socket and tongue and grooved faces (see Fig. 14.23c), the gasket is confined in a groove, which prevents failure by "blow-out." Matched pairs of flanges are required, which increases the cost, but this type is suitable for high-pressure and high-vacuum service. Ring joint flanges (Fig. 14.23d) are used for high-temperature and high-pressure services.

14.10.4 Flange design

Standard flanges will be specified for most applications (see Section 14.10.5). Special designs would be used only if no suitable standard flange were available or for large flanges, such as the body flanges of vessels, where it may be cheaper to size a flange specifically for the duty required rather than to accept the nearest standard flange, which of necessity would be oversized.

Fig. 14.24 shows the forces acting on a flanged joint. The bolts hold the faces together, resisting the forces due to the internal pressure and the gasket sealing pressure. As these forces are offset, the flange is subjected to a bending moment. It can be considered a cantilever beam with a concentrated load. A flange assembly must be sized so as to have sufficient strength and rigidity to resist this bending moment. A flange that lacks sufficient rigidity will rotate

TABLE 14.4 Gasket materials (based on Table 2-5.1 in ASME BPV Code Sec. VIII D.1 Mandatory Appendix 2 and a similar table in BS 5500—2003)

Gasket Material		Gasket Factor m	Min.Design Seating Stress y(N/mm^2)	Sketches	Minimum Gasket Width (mm)
Rubber without fabric or a high percentage of asbestos fiber; hardness:					
below 75° IRH		0.50	0		10
75° IRH or higher		1.00	14		
Asbestos with a suitable binder for the operating conditions	3.2 mm thick	2.00	11.0		
	1.6 mm thick	2.75	25.5		10
	0.8 mm thick	3.50	44.8		
Rubber with cotton fabric insertion		1.25	2.8		10
Rubber with asbestos fabric insertion, with or without wire reinforcement	3-ply	2.25	15.2		
	2-ply	2.50	20.0		10
	1-ply	2.75	25.5		
Vegetable fiber		1.75	7.6		10
Spiral-wound metal, asbestos filled	Carbon	2.50	20.0		
	Stainless steel	3.00	31.0		10
Corrugated metal, asbestos inserted	Soft aluminum	2.50	20.0		
	Soft copper or brass	2.75	25.5		
or	Iron or soft steel	3.00	31.0		10
Corrugated metal, jacketed asbestos filled	Monel or 4 to 6% chrome	3.25	37.9		
	Stainless steels	3.50	44.8		
	Soft aluminum	2.75	25.5		
	Soft copper or brass	3.00	31.0		
Corrugated metal	Iron or soft steel	3.25	37.9		10
	Monel or 4 to 6% Chrome	3.50	44.8		
	Stainless steels	3.75	52.4		
	Soft aluminum	3.25	37.9		
	Soft copper or brass	3.50	44.8		
Flat metal jacketed asbestos filled	Iron or soft steel	3.75	52.4		
	Monel	3.50	55.1		10
	4 to 6% chrome	3.75	62.0		
	Stainless steels	3.75	62.0		
	Soft aluminum	3.25	37.9		
	Soft copper or brass	3.50	44.8		
Grooved metal	Iron or soft steel	3.75	52.4		10
	Monel or 4 to 6% chrome	3.75	62.0		
	Stainless steels	4.25	69.5		
	Soft aluminum	4.00	60.6		
	Soft copper or brass	4.75	89.5		
Solid flat metal	Iron or soft steel	5.50	124		6
	Monel or 4 to 6% chrome	6.00	150		
	Stainless steels	6.50	179		
Ring joint	Iron or soft steel	5.50	124		
	Monel or 4 to 6% chrome	6.00	150		6
	Stainless steels	6.50	179		

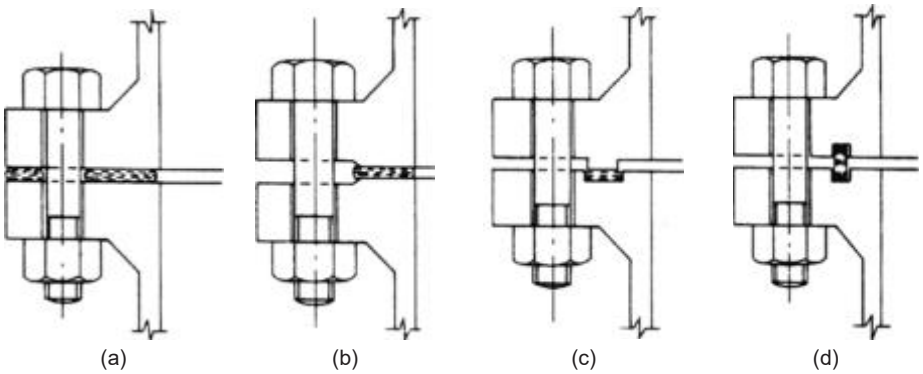


FIG. 14.23 Flange types and faces. (a) Full face. (b) Gasket within bolt circle. (c) Spigot and socket. (d) Ring-type joint.

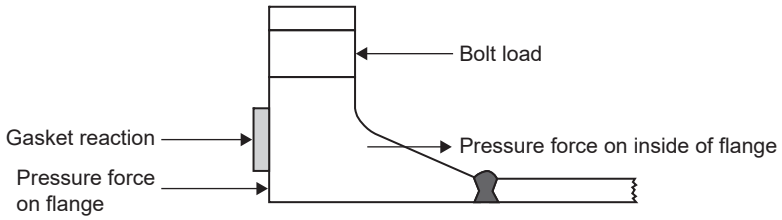


FIG. 14.24 Forces acting on an integral flange.

slightly, and the joint will leak (Fig. 14.25). The principles of flange design are discussed by Singh and Soler (1992) and Azbel and Cheremisinoff (1982). Singh and Soler give a computer program for flange design. Design procedures for pressure vessel flanges are given in ASME BPV Code Sec VIII D.1 Mandatory Appendix 2.

For design purposes, flanges are classified as integral or loose flanges. Integral flanges are those in which the construction is such that the flange obtains support from its hub and the connecting nozzle (or pipe). The flange assembly and nozzle neck form an "integral" structure. A welding-neck flange would be classified as an integral flange. Loose flanges are attached to the nozzle (or pipe) in such a way that they obtain no significant support from the nozzle neck and cannot be classified as an integral attachment. Screwed and lap-joint flanges are typical examples of loose flanges.

The number of bolts and the bolt size must be chosen such that the bolt load is less than the maximum allowable stress in the bolts. The bolt spacing must be selected to give a uniform compression of the gasket. It will not normally be less than 2.5 times the bolt diameter to give sufficient clearance for tightening with a wrench. The following formula can be used to determine the maximum bolt spacing:

$$p_b = 2d_b + \frac{6t_f}{(m + 0.5)} \tag{14.49}$$

where p_b = bolt pitch (spacing), mm,
d_b = bolt diameter, mm,
t_f = flange thickness, mm,
m = gasket factor.

Bolting requirements are given in ASME B16.5. An overview of the B16.5 requirements is given by Stikvoort (2019).

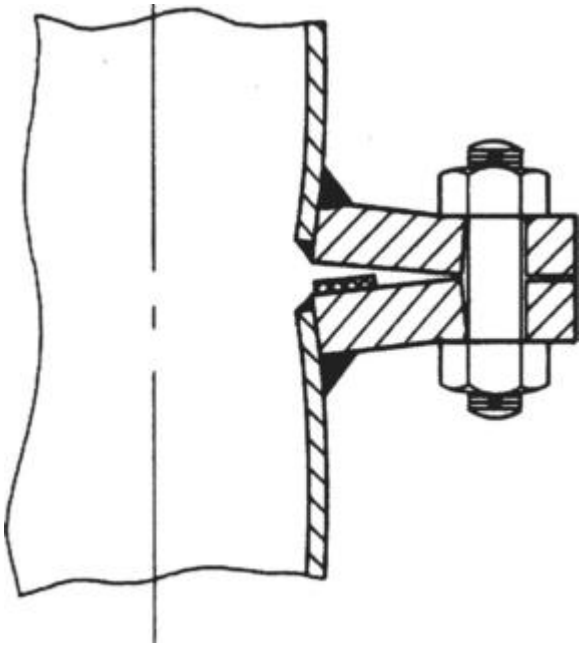
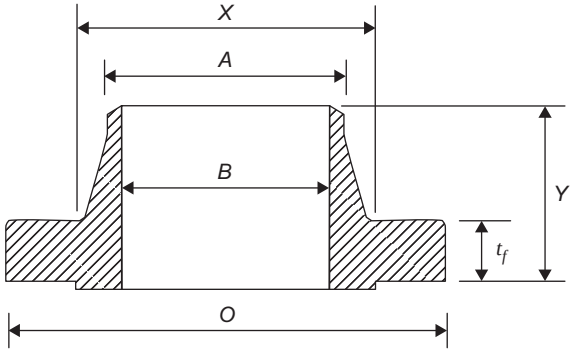


FIG. 14.25 Deflection of a weak flange (exaggerated).



Flange class	Nominal pipe size	Outside diameter of flange, *O*	Thickness of flange, t_f	Diameter of hub, *X*	Diameter beginning of chamfer, *A*	Length through hub, *Y*	Bore, *B*
150	1.00	4.25	0.50	1.94	1.32	2.12	1.05
	2.00	6.00	0.69	3.06	2.38	2.44	2.07
	4.00	9.00	0.88	5.31	4.50	2.94	4.03
	6.00	11.00	0.94	7.56	6.63	3.44	6.07
	8.00	13.50	1.06	9.69	8.63	3.94	7.98
	12.00	19.00	1.19	14.38	12.75	4.44	12.00
	24.00	32.00	1.81	26.12	24.00	5.94	TBS
300	1.00	4.88	0.62	2.12	1.32	2.38	1.05
	2.00	6.50	0.81	3.31	2.38	2.69	2.07
	4.00	10.00	1.19	5.75	4.50	3.32	4.03
	6.00	12.50	1.38	8.12	6.63	3.82	6.07
	8.00	15.00	1.56	10.25	8.63	4.32	7.98
	12.00	20.50	1.94	14.75	12.75	5.06	12.00
	24.00	36.00	2.69	27.62	24.00	6.56	TBS

Note: TBS = To be specified by purchaser.

FIG. 14.26 Standard flange dimensions for welding neck flanges based on ASME B16.5 Annex F.

14.10.5 Standard flanges

Standard flanges are available in a range of types, sizes, and materials and are used extensively for pipes, nozzles, and other attachments to pressure vessels.

Standards for flanges and pipe fittings are set by the ASME B16 committee. These include:

ASME B16.5	Pipe flanges and flanged fittings
ASME B16.9	Factory-made wrought buttwelding fittings
ASME B16.11	Forged fittings, socket-welding and threaded
ASME B16.15	Cast bronze threaded fittings
ASME B16.24	Cast copper alloy pipe flanges and flanges fittings
ASME B16.42	Ductile iron pipe flanges and flanges fittings
ASME B16.47	Large diameter steel flanges

An abstract of the American standards is given by Green and Southard (2018).

A typical example of a standard flange design is shown in Fig. 14.26. This was based on information in ASME B16.5 Annex F.

Standard flanges are designated by class numbers, or rating numbers, which roughly correspond to the primary service (pressure) rating of a steel flange of those dimensions at room temperature.

The flange class number required for a particular application will depend on the design pressure and temperature and the material of construction. The reduction in strength at elevated temperatures is allowed for by selecting a flange with a higher rating than the design pressure. For example, for a design pressure of 10 bar (150 psi), a class 150 flange would be selected for a service temperature below 300 °C, whereas for a service temperature of, say, 300 °C a 300-pound flange would be specified. A typical pressure–temperature relationship for carbon steel flanges is shown in Table 14.5. Pressure–temperature ratings for a full range of materials can be obtained from the design codes.

Designs and dimensions of standard flanges over the full range of pipe sizes are given in ASME B16.5 Annex F. A summary of flange dimensions is given by Green and Southard (2018), which can be used for preliminary designs. The current standards and suppliers' catalogues should be consulted before firming up the design.

TABLE 14.5 Typical pressure–temperature ratings for carbon steel flanges, A350, A515, A516

	Working pressure by flange class (psig)						
Temperature	**150**	**300**	**400**	**600**	**900**	**1500**	**2500**
−20 to 100	285	740	985	1480	2220	3705	6170
200	260	680	905	1360	2035	3395	5655
300	230	655	870	1310	1965	3270	5450
400	200	635	845	1265	1900	3170	5280
500	170	605	805	1205	1810	3015	5025
600	140	570	755	1135	1705	2840	4730
700	110	530	710	1060	1590	2655	4425
800	80	410	550	825	1235	2055	3430

Adapted from ASME B16.5 Annex F Table F2-1.1.

14.11 Welded joint design

Process vessels are built up from preformed parts: cylinders, heads, and fittings, joined by fusion welding. Riveted construction was used extensively in the past (before the 1940s) but is now rarely seen except on very old plants.

Cylindrical sections are usually made up from plate sections rolled to the required curvature. The sections (strakes) are made as large as is practicable to reduce the number of welds required. The longitudinal welded seams are offset to avoid a conjunction of welds at the corners of the plates.

Many different forms of welded joints are needed in the construction of a pressure vessel. Some typical forms are shown in Figs. 14.27 to 14.29.

The design of a welded joint should satisfy the following basic requirements:

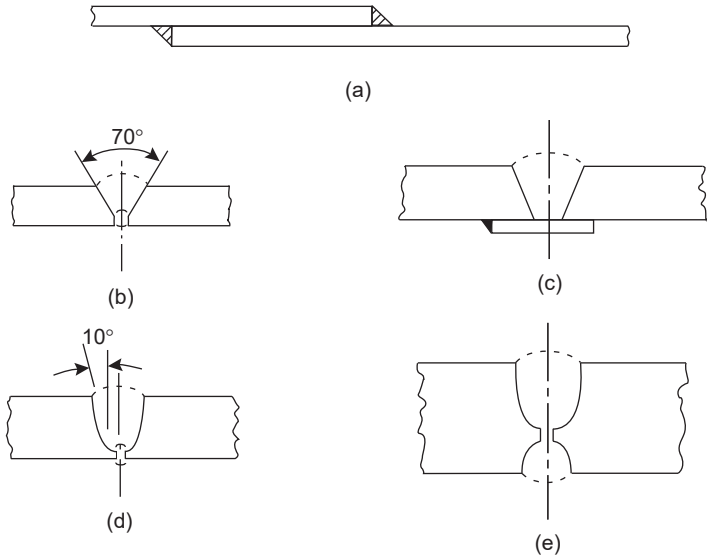


FIG. 14.27 Weld profiles (b to e) butt welds. (a) Lap joint. (b) Single "V." (c) Backing strip. (d) Single "U." (e) Double "U."

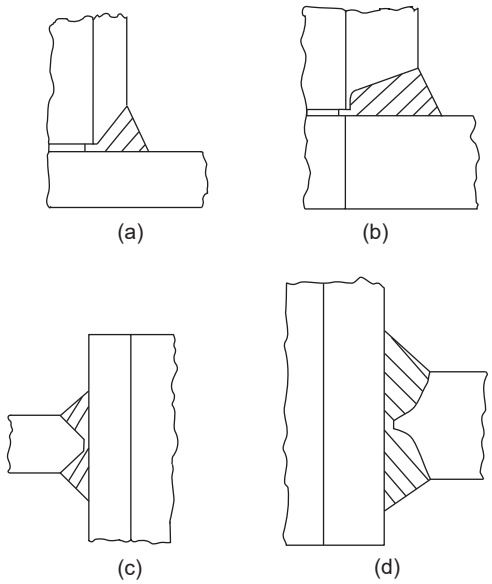


FIG. 14.28 Typical weld profiles. (a), (b) Branches. (c) Set-on branches. (d) Set-in branches.

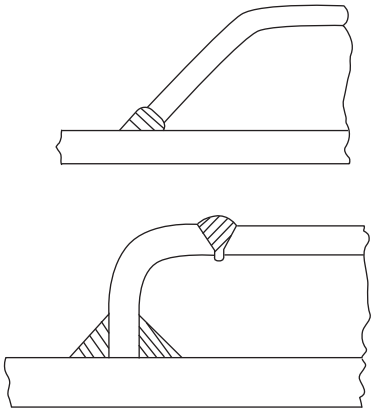


FIG. 14.29 Typical construction methods for welded jackets.

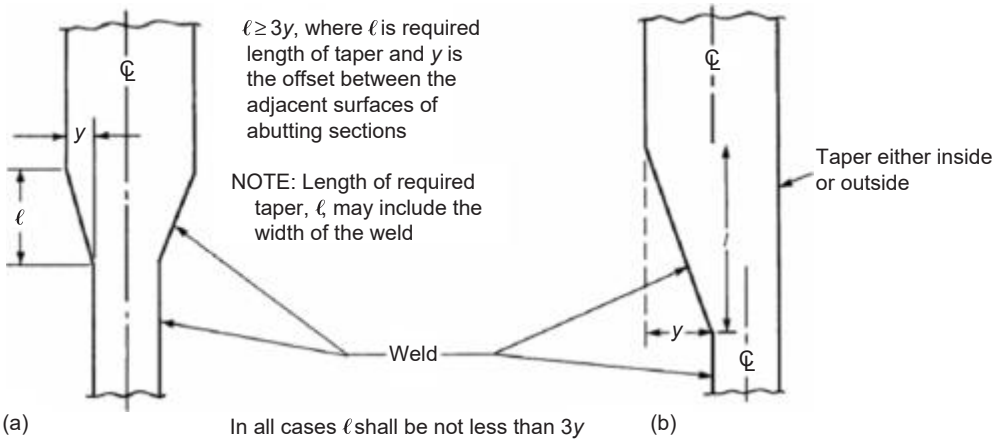


FIG. 14.30 Butt welding of plates of unequal thickness. *Reprinted from ASME 2004 BPVC, Section VIII-Div.1 by permission of the American Society of Mechanical Engineers. All rights reserved.*

1. Give good accessibility for welding and inspection.
2. Require the minimum amount of weld metal.
3. Give good penetration of the weld metal, from both sides of the joint, if practicable.
4. Incorporate sufficient flexibility to avoid cracking due to differential thermal expansion.

The preferred types of joints, and recommended designs and profiles, are given in the codes and standards. See, for example, ASME BPV Code Sec. VIII D.1, Part UW − Requirements for pressure vessels fabricated by welding.

The correct form to use for a given joint will depend on the material, the method of welding (machine or hand), the plate thickness, and the service conditions. Double-sided V- or U-sections are used for thick plates and single V- or U-profiles for thin plates. A backing strip is used where it is not possible to weld from both sides. Lap joints are seldom used for pressure vessel construction, but are used for atmospheric pressure storage tanks.

Where butt joints are made between plates of different thicknesses, the thicker plate is reduced in thickness with a slope of not greater than 1 in 3 (19 degrees) (ASME BPV Code Sec. VIII D.1 Part UW-9, shown in Fig. 14.30).

The local heating, and consequent expansion that occurs during welding can leave the joint in a state of stress. These stresses are relieved by postwelding heat treatment. Not all vessels will be stress relieved. Guidance on the need for postwelding heat treatment is given in ASME BPV Code Sec. VIII D.1 Part UW-40 and will depend on the service and conditions, materials of construction, and plate thickness.

To ensure that a satisfactory quality of welding is maintained, welding machine operators and welders working on the pressure parts of vessels are required to pass welder approval tests, which are designed to test their competence to make sound welds. Welding and brazing qualifications are discussed in Section IX of the ASME BPV Code.

14.12 Fatigue assessment of vessels

During operation, the shell or components of the vessel may be subjected to cyclic stresses. Stress cycling can arise from the following causes:

1. Periodic fluctuations in operating pressure
2. Temperature cycling
3. Vibration
4. "Water hammer"
5. Fluctuations in the flow of fluids or solids
6. Periodic fluctuation of external loads

A detailed fatigue analysis is required if any of these conditions is likely to occur to any significant extent. Fatigue failure will occur during the service life of the vessel if the endurance limit (number of cycles for failure) at the particular value of the cyclic stress is exceeded. The codes and standards should be consulted to determine when a detailed fatigue analysis must be undertaken.

14.13 Pressure tests

The pressure vessel codes and standards require that all pressure vessels be subjected to a pressure test to prove the integrity of the finished vessel (ASME BPV Code Sec. VIII D.1 Part UG-99). A hydraulic test is normally carried out, but a pneumatic test can be substituted under circumstances where the use of a liquid for testing is not practical. Hydraulic tests are safer because only a small amount of energy is stored in the compressed liquid. A standard pressure test is used when the required thickness of the vessel parts can be calculated in accordance with the particular code or standard. The vessel is tested at a pressure 30% above the design pressure. The test pressure is adjusted to allow for the difference in strength of the vessel material at the test temperature compared with the design temperature and for any corrosion allowance.

Formulae for determining the appropriate test pressure are given in the codes and standards; typically:

$$\text{Test pressure} = 1.30 \left[P_d \frac{S_a}{S_n} \times \frac{t}{(t-c)} \right] \tag{14.50}$$

where P_d = design pressure, N/mm^2
S_a = maximum allowable stress at the test temperature, N/mm^2
S_n = maximum allowable stress at the design temperature, N/mm^2
c = corrosion allowance, mm
t = actual plate thickness, mm

When the required thickness of the vessel component parts cannot be determined by calculation in accordance with the methods given, the ASME BPV Code requires that a hydraulic proof test be carried out (Sec. VIII D.1 Part UG-101). In a proof test the stresses induced in the vessel during the test are monitored using strain gauges or similar techniques. In a proof test a duplicate of the vessel or part is tested until the part yields or bursts. The requirements for the proof testing of vessels are set out in ASME BPV Code Sec. VIII D.1 Part UG-101.

14.14 High-pressure vessels

High pressures are required for many commercial chemical processes. For example, the synthesis of ammonia is carried out at reactor pressures of up to 1000 bar, and high-density polyethylene processes operate up to 1500 bar.

Although there is no prescribed upper limit on pressure for vessels designed in accordance with ASME BPV Code Section VIII Division 1, the rules given in that section of the code usually cannot be economically satisfied for vessels designed to operate above 3000 psia (200 bar). For pressures greater than about 2000 psia, the alternative rules given in Section VIII Division 2 will usually lead to a more economical design. Division 2 restricts the materials that can be used, the allowable operating temperatures (not greater than 900 °F) and places stricter requirements on stress analysis and testing. The additional engineering and design costs are usually justified for high-pressure vessels because the Division 2 rules allow higher maximum allowable stresses and hence lead to thinner-walled vessels.

At the highest operating pressures, typically above 10,000 psia (680 bar), the alternative design rules given in ASME BPV Code Section VIII Division 3 can be followed.

A full discussion of the design and construction of high-pressure vessels and ancillary equipment (pumps, compressors, valves, and fittings) is given in the books by Fryer and Harvey (1997) and Jawad and Farr (2018). At high pressures it becomes increasingly difficult to fabricate single-walled vessels with sufficient strength because of the wall thickness and depth of welds required. Instead, compound vessels with several layers of vessel walls are often used. In a compound vessel, the outer layers can be used to place the inner layers in compression during manufacture, and hence offset the tensile forces that will act most strongly on the inner layers during operation.

14.14.1 Compound vessels

Shrink-fitted cylinders

Compound vessels can be made by shrinking one cylinder over another. The inside diameter of the outer cylinder is made slightly smaller than the outer diameter of the inner cylinder and is expanded by heating to fit over the inner. On cooling, the outer cylinder contracts and places the inner under compression. The stress distribution in a two-cylinder compound vessel is shown in Fig. 14.31; more than two cylinders may be used.

Shrink-fitted compound cylinders are used for small-diameter vessels, such as compressor cylinder barrels. The design of shrink-fitted compound cylinders is discussed by Manning (1947) and Jawad and Farr (2018).

Multilayer vessels

Multilayer vessels are made by wrapping several layers of relatively thin plate round a central tube. The plates are heated, tightened, and welded, and this gives the desired stress distribution in the compound wall. The vessel is closed with forged heads. A typical design is shown in Fig. 14.32. This construction technique is discussed by Jasper and Scudder (1941) and Jawad and Farr (2018).

Wound vessels

Cylindrical vessels can be reinforced by winding on wire or thin ribbons. Winding on the wire under tension places the cylinder under compression. For high-pressure vessels special interlocking strips are used, such as those shown in Fig. 14.33. The interlocking gives strength in the longitudinal direction and a more uniform stress distribution. The strips may be wound on hot to increase the pre-stressing. This type of construction is described by Birchall and Lake (1947).

14.14.2 Autofrettage

Autofrettage is a technique used to prestress the inner part of the wall of a monobloc vessel to give a similar stress distribution to that obtained in a shrink-fitted compound cylinder. The finished vessel is deliberately overpressurized by hydraulic pressure. During this process, the inner part of the wall will be more highly stressed than the outer part and will undergo plastic strain. On release of the "autofrettage" pressure, the inner part, which is now oversized, will be placed under compression by the elastic contraction of the outer part, which gives a residual stress distribution similar to that obtained in a two-layer, shrink-fitted compound cylinder. After straining, the vessel is annealed at a relatively low temperature, approximately 300 °C. The straining also work-hardens the inner part of the wall. The vessel can be used at pressures up to the "autofrettage" pressure without further permanent distortion. The autofrettage technique is discussed by Manning (1950) and Jawad and Farr (2018).

Requirements for pressure vessels fabricated by layered construction are given in ASME BPV Code Sec. VIII D.1 Part ULW and Sec. VIII D.2 Articles D-11 and F-8.

14.15 Liquid storage tanks

Vertical cylindrical tanks, with flat bases and conical roofs, are universally used for the bulk storage of liquids at atmospheric pressure. Tank sizes vary from a few hundred gallons (tens of cubic meters) to several thousand gallons (several hundred cubic meters).

The main load to be considered in the design of these tanks is the hydrostatic pressure of the liquid, but the tanks must also be designed to withstand wind loading and, for some locations, the weight of snow on the tank roof.

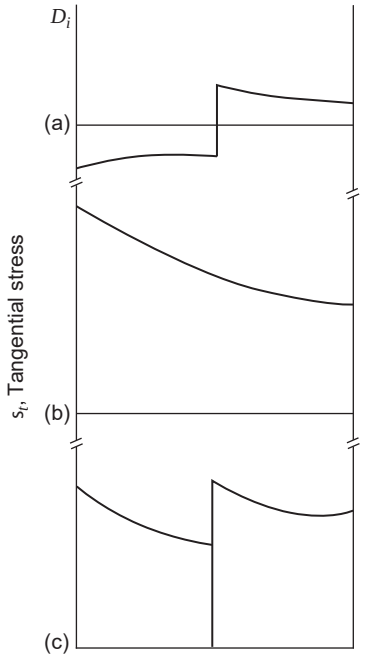


FIG. 14.31 Stress distribution in a shrink-fitted compound cylinder. (a) Due to shrinkage. (b) Due to pressure. (c) Combined (a + b).

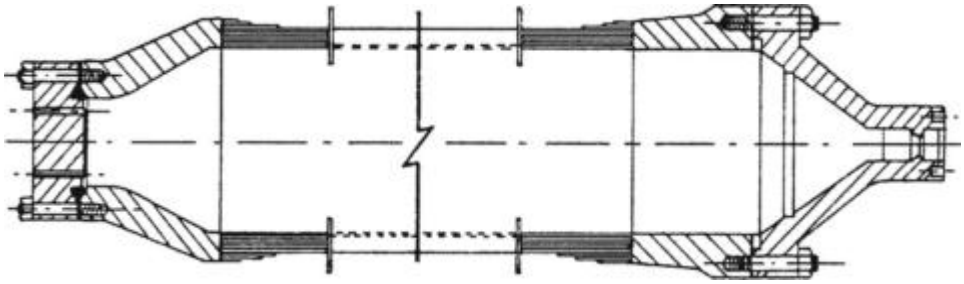


FIG. 14.32 Multilayer construction.

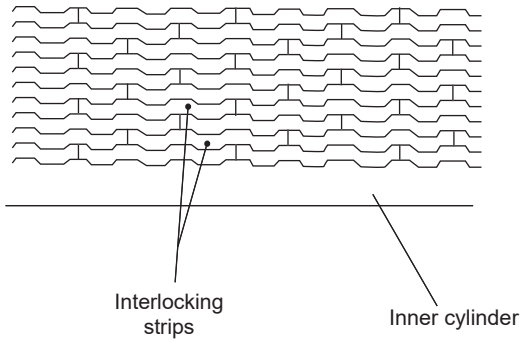


FIG. 14.33 Strip-wound vessel.

The minimum wall thickness required to resist the hydrostatic pressure can be calculated from the equations for the membrane stresses in thin cylinders (Section 14.3.4):

$$t_t = \frac{\rho_L H_L g}{2 S_t E} \frac{D_t}{10^3} \tag{14.51}$$

where t_t = tank thickness required at depth H_L, mm
H_L = liquid depth, m
ρ_L = liquid density, kg/m^3
E = joint efficiency (if applicable)
g = gravitational acceleration, 9.81 m/s^2
S_t = maximum allowable stress for tank material, N/mm^2
D_t = tank diameter, m

The liquid density should be taken as that of water (1000 kg/m^3), unless the process liquid has a greater density.

For small tanks, a constant wall thickness would normally be used, calculated at the maximum liquid depth. With large tanks, it is economical to take account of the variation in hydrostatic pressure with depth by increasing the plate thickness progressively from the top to bottom of the tank. Plate widths of 2 m (6 ft) are typically used in tank construction.

The roofs of large tanks need to be supported by a steel framework supported on columns in very large-diameter tanks.

The design and construction of atmospheric storage tanks for the petroleum industry are covered by the American Petroleum Industry standards API 650 (2003) and 620 (2002). Other standards are also used internationally, for example, British Standard BS 2654 and BS EN 14015 for larger steel tanks and European Standard EN 13121 for glass-reinforced polymer tanks. The design of storage tanks is covered in the books by Myers (1997) and Jawad and Farr (2018). See also the papers by Debham et al. (1968) and Zick and McGrath (1968).

14.16 Capital cost of pressure vessels

The purchased equipment cost of a pressure vessel depends strongly on the complexity of the design. Preliminary costing methods will usually only generate very approximate answers, and consultation with a vessel manufacturer will be needed to firm up the estimate. Pressure vessels are often the most expensive pieces of equipment in a chemical plant. Vessels for high pressures (above 100 bar) will often be designed in accordance with the ASME BPV Code Section VIII Div.2 and may have long lead times because of the relative scarcity of fabricators that are qualified for Division 2 construction.

Most preliminary cost correlations for pressure vessels are based on the shell mass, so it is necessary to know the wall thickness as well as the general dimensions of the vessel. Wall thickness can be estimated using the BPV Code equations given in Section 14.5 and the combined loading analysis given in Section 14.8. It is very important to specify the design pressure and temperature correctly in these calculations. The choice of material of construction plays a key role in determining the wall thickness (through the maximum allowable stress and corrosion allowance), as well as affecting the cost through the materials cost factor. Preliminary cost correlations are discussed in Section 7.5.2, and correlations for pressure vessel costs are given in Table 7.2. The use of these correlations for costing horizontal and vertical pressure vessels is illustrated in Example 7.3.

Simple cost correlations cannot address any complexity in the design of a pressure vessel. If the vessel contains substantial internal features, has a large number of ports or manifolds, or requires stiffening rings to handle vacuum operation, then costs for these features must be added to the bare vessel cost.

More accurate cost estimates for pressure vessels are made by determining the parts and materials cost and fabrication work breakdown structure, and then assigning costs based on estimates of the labor and machine time required for vessel construction; see Section 7.5.3. This is the method used in the Aspen Capital Cost Estimator cost estimating software. Reasonably good estimates of pressure vessel costs can be obtained using commercial cost estimating programs if the design engineer is careful in specifying the vessel design conditions.

14.17 References

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14.18 Nomenclature

Note that the same nomenclature has been used as in the ASME BPV Code and API recommended practices and standards as far as possible. This occasionally causes the same symbol to be used with different meanings in different contexts. Where the context is not clear and there is a possibility of confusion, a new symbol has been assigned.

		Dimensions in MLT
a_e	Acceleration due to an earthquake	$\mathbf{LT}^{-2}$
C	Constant in Equation 14.16	—
C_d	Drag coefficient in Equation 14.36	—
C_e	Seismic constant	—
C_w	Weight factor in Equation 14.32	—
c	Corrosion allowance	**L**
D	Diameter	**L**
D_c	Diameter of cone at point of interest	**L**
D_e	Nominal diameter of flat end	**L**
D_{eff}	Effective diameter of column for wind loading	**L**
D_i	Internal diameter	**L**
D_m	Mean diameter	**L**
D_o	Outside diameter	**L**
D_s	Skirt internal diameter	**L**
D_t	Tank diameter	**L**
d_b	Bolt diameter	**L**
E	Joint efficiency, welded joint	—

		Dimensions in MLT
E_Y	Young's modulus	$\mathbf{ML^{-1}T^{-2}}$
F_{bs}	Load supported by bracket	$\mathbf{MLT^{-2}}$
F_L	Force in longitudinal (vertical) direction	$\mathbf{MLT^{-2}}$
F_p	Local, concentrated, wind load	$\mathbf{MLT^{-2}}$
F_s	Shear force due to an earthquake	$\mathbf{MLT^{-2}}$
F_v	Force in horizontal direction	$\mathbf{MLT^{-2}}$
g	Gravitational acceleration	$\mathbf{LT^{-2}}$
H_L	Liquid depth	$\mathbf{L}$
H_p	Height of local load above base	$\mathbf{L}$
H_v	Height (length) of cylindrical section between tangent lines	$\mathbf{L}$
I_p	Polar second moment of area	$\mathbf{L^4}$
I_v	Second moment of area of vessel	$\mathbf{L^4}$
L	Unsupported length of vessel	$\mathbf{L}$
L_d	Bracket depth	$\mathbf{L}$
L_o	Distance between center line of equipment and column	$\mathbf{L}$
M	Bending moment	$\mathbf{ML^2T^{-2}}$
M_e	Bending moment due to offset equipment	$\mathbf{ML^2T^{-2}}$
M_p	Bending moment at base due to local load	$\mathbf{ML^2T^{-2}}$
M_s	Bending moment at base of skirt	$\mathbf{ML^2T^{-2}}$
M_x	Bending moment at point x from free end of column	$\mathbf{ML^2T^{-2}}$
m	Gasket factor	—
P_d	Design pressure	$\mathbf{ML^{-1}T^{-2}}$
P_i	Internal pressure	$\mathbf{ML^{-1}T^{-2}}$
P_w	Wind pressure loading	$\mathbf{ML^{-1}T^{-2}}$
P_b	Bolt pitch	$\mathbf{L}$
R_c	Crown radius	$\mathbf{L}$
R_k	Knuckle radius	$\mathbf{L}$
R_p	Radius of curvature of plate	$\mathbf{L}$
S	Maximum allowable stress (design stress)	$\mathbf{ML^{-1}T^{-2}}$
S_a	Maximum allowable stress at test temperature	$\mathbf{ML^{-1}T^{-2}}$
S_n	Maximum allowable stress at design temperature	$\mathbf{ML^{-1}T^{-2}}$
S_s	Maximum allowable stress for skirt material	$\mathbf{ML^{-1}T^{-2}}$
S_t	Maximum allowable stress for tank material	$\mathbf{ML^{-1}T^{-2}}$
T	Torque	$\mathbf{ML^{-1}T^{-2}}$
t	Thickness of plate or shell	$\mathbf{L}$
t_c	Thickness of bracket plate	$\mathbf{L}$
t_f	Thickness of flange	$\mathbf{L}$
t_s	Thickness of shell	$\mathbf{L}$
t_{sk}	Skirt thickness	$\mathbf{L}$

		Dimensions in MLT
t_t	Tank wall thickness	**L**
u_w	Wind velocity	$\mathbf{LT}^{-1}$
W	Wind load per unit length	$\mathbf{MT}^{-2}$
W_e	Weight of ancillary equipment	$\mathbf{MLT}^{-2}$
W_v	Weight of vessel and contents	$\mathbf{MLT}^{-2}$
W_z	Weight of vessel and contents above a plane at elevation z	$\mathbf{MLT}^{-2}$
x	Distance from free end of cantilever beam	**L**
y	Minimum seating pressure for gasket	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
α	Half cone apex angle	—
θ_s	Base angle of conical section	—
ν	Poisson's ratio	—
ρ_m	Density of vessel material	$\mathbf{ML}^{-3}$
ρ_a	Density of air	$\mathbf{ML}^{-3}$
ρ_L	Liquid density	$\mathbf{ML}^{-3}$
σ	Normal stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_b	Bending stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_{bs}	Bending stress in skirt	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_c	Critical buckling stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_e	Stress at elastic limit of material	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ'_e	Elastic limit stress divided by factor of safety	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_h	Circumferential (hoop) stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_L	Longitudinal stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_s	Stress in skirt support	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_w	Stress due to weight of vessel	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_{ws}	Stress in skirt due to weight of vessel	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_x	Normal stress in x direction	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_y	Normal stress in y direction	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_z	Axial stresses in vessel	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_1, σ_2, σ_3	Principal stresses	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
τ	Torsional shear stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
τ_e	Shear stress at elastic limit of material	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
τ_{xy}	Shear stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
τ_1, τ_2, τ_3	Shear stress maxima	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
Superscript		
^	Maximum	

14.19 Problems

14.1. A horizontal, cylindrical tank with hemispherical ends is used to store liquid chlorine at 10 bar. The vessel is 4 m internal diameter and 20 m long. Estimate the minimum wall thickness required to resist this pressure for the cylindrical section and the heads. Take the design pressure as 12 bar and the maximum allowable stress for the material as 110 MN/m^2.

14.2. The thermal design of a heat exchanger to recover heat from a kerosene stream by transfer to a crude oil stream was in Chapter 19, Example 19.2. Make a preliminary mechanical design for this exchanger. Base your design on the specification obtained from the CAD design procedure used in the example. All material of construction to be carbon steel (semi-killed or silicon killed). Your design should cover:

a. Choice of design pressure and temperature
b. Choice of the required corrosion allowances
c. Choice of the type of end covers
d. Determination of the minimum wall thickness for the shell, headers, and ends
e. A check on the pressure rating of the tubes

14.3. Make a preliminary mechanical design for the vertical thermosyphon reboiler for which the thermal design was done as Example 19.9 in Chapter 19. The inlet liquid nozzle and the steam connections will be 50 mm inside diameter. Flat plate end closures will be used on both headers. The reboiler will be hung from four bracket supports, positioned 0.5 m down from the top tube plate. The shell and tubes will be of semi-killed carbon steel. Your design should cover:

a. Choice of design pressure and temperature
b. Choice of the required corrosion allowances
c. Selection of the header dimensions
d. Determination of the minimum wall thickness for the shell, headers, and ends
e. A check on the pressure rating of the tubes

14.4. The specification for a sieve plate column is given here. Make a preliminary mechanical design for the column. Your design should include:

a. Column wall thickness
b. Selection and sizing of vessel heads
c. The nozzles and flanges (use standard flanges)
d. Column supporting skirt

You need not design the plates or plate supports.
You should consider the following design loads:

a. Internal pressure
b. Wind loading
c. Dead weight of vessel and contents (vessel full of water)

There will be no significant loading from piping and external equipment. Earthquake loading need not be considered.
Column specification:

Length of cylindrical section, 37 m
Internal diameter, 1.5 m
Heads, standard ellipsoidal
50 sieve plates
Nozzles: feed, at mid-point, 50 mm inside diameter
vapor out, 0.7 m below top of cylindrical section, 250 mm inside diameter
bottom product, center of vessel head, 50 mm inside diameter
reflux return, 1.0 m below top of cylindrical section, 50 mm inside diameter
Two 0.6-m-diameter access ports (manholes) situated 1.0 m above the bottom and 1.5 m below the top of the column
Support skirt height, 2.5 m
Access ladder with platforms
Insulation, mineral wool, 50 mm thick

Materials of construction: vessel stainless steel, unstabilized (304)
nozzles as vessel
skirt carbon steel, silicon killed
Design pressure 1200 kN/m^2
Design temperature 150 °C
Corrosion allowance, 2 mm

Make a dimensioned sketch of your design and fill out the column specification sheet given in Appendix G (available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793).

14.5. A fixed-bed reactor is to be designed for a hydrocracking process. The reactor will treat 320,000 lb/h of vacuum gas oil (specific gravity 0.85) in the presence hydrogen at 650 °F, 2000 psig, 1.0 weight hourly space velocity (WHSV). The catalyst has bulk density of 50 lb/ft^3 and void fraction 0.4. The catalyst is to be divided into four beds to allow a hydrogen quench to be brought in between the beds for temperature control. Make a preliminary mechanical design of the reactor(s). Your design should include:

a. Selection of material of construction
b. Sizing of the vessel(s), including allowance for any internals
c. Determination of the required wall thickness
d. Selection and sizing of vessel heads
e. The nozzles and flanges (use standard flanges)
f. A support skirt

You need not design the vessel internals.
You should consider the following design loads:

a. Internal pressure
b. Wind loading
c. Dead weight of vessel and contents (vessel full of catalyst and gas oil)
d. Hydraulic testing with no catalyst and vessel full of water

14.6. A jacketed vessel is to be used as a reactor. The vessel has an internal diameter of 2 m and is fitted with a jacket over a straight section 1.5 m long. Both the vessel and jacket walls are 25 mm thick. The spacing between the vessel and jacket is 75 mm.
The vessel and jacket are made of carbon steel. The vessel will operate at atmospheric pressure, and the jacket will be supplied with steam at 20 bar. Check if the thickness of the vessel and jacket is adequate for this duty. Take the allowable design stress as 100 N/mm^2 and the value of Young's modulus at the operating temperature as 180,000 N/mm^2.

14.7. A storage tank for concentrated nitric acid will be constructed from aluminum to resist corrosion. The tank is to have an inside diameter of 6 m and a height of 17 m. The maximum liquid level in the tank will be at 16 m. Estimate the plate thickness required at the base of the tank. Take the allowable design stress for aluminum as 90 N/mm^2.

CHAPTER

15

Design of reactors and mixers

KEY LEARNING OBJECTIVES

- How to select and size a reactor
- Factors to consider in optimizing reaction conditions
- How to design mixers
- How to design reactors for heating, cooling, and catalysis
- How to design reactors for multiphase reactions
- How to design reactors for biological processes
- Factors to consider in scaling up reactions from the laboratory to plant scale

15.1 Introduction

The reactor is the heart of a chemical process, where chemical reactions are carried out to transform feeds into products. Reactors are usually designed as special items for a given project. Many reactor designs are unique and proprietary, particularly when the reaction system involves catalysis or multiphase flow. Even conventional stirred tanks are often customized for the application by optimization of internal mixing pattern, feed addition points, heat transfer surface, or control instrumentation.

Numerous textbooks have been published on the subjects of chemical kinetics and reaction engineering, and a selection is given in the bibliography at the end of this chapter. These subjects will not be covered here. Instead, the focus will be on translating the reactor design parameters into process equipment specifications that can be used to lay out a preliminary reactor design and develop drawings and specifications for use by detailed equipment design groups.

Reactor design is a vital step in the overall design of the process, and it is important to ensure that the equipment specified will be capable of achieving the desired yields and selectivity when operated at full scale. Few industrial reactors are designed solely based on detailed modeling of the kinetics and hydrodynamics; instead, reactors are usually scaled up from pilot plant reactors or previous designs, making suitable allowance for heat transfer, mass transfer, residence time, or whatever other parameters have been determined to govern the size. The final volume of real reactors is often determined more by the needs for mixing, segregation, or heat transfer than by the residence time required for the reaction.

15.2 Reactor design: General procedure

This section provides a generalized overall procedure for reactor design that applies to most reacting systems. Further information on the steps in this procedure will be given in subsequent sections.

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15.2.1 General procedure for reactor design

The design of a chemical reactor should not be carried out in isolation from overall process design. It will usually be necessary to determine optimal conditions of reactor conversion, selectivity, and yield of by-products, as described in Chapter 2. Optimization of the reactor performance thus requires a design of the process separations and heat recovery, as well as costing and economic analysis. Although the reactor itself is usually a relatively small fraction of the process fixed capital cost, the reactor performance can have a very significant impact on capital and operating costs elsewhere in the process.

The design of a reactor should therefore begin with an overall process design to set rough targets for yield and selectivity, as discussed in Sections 2.3.3 and 2.6.1. At this stage, there may be very little reaction kinetics information available; indeed, it is very unlikely that there will be sufficient information to develop a model that accurately predicts the effect of feed contaminants and the formation of by-products. All that the designer needs at this point is a rough idea of what yields are feasible in a given residence time or space velocity; a few good data points from the laboratory are usually sufficient to get started.

The overall procedure for reactor design is given in Fig. 15.1. The steps in this procedure are described next. During several of the steps it may be necessary for the design engineer to interact with researchers to collect additional data, as indicated in the figure.

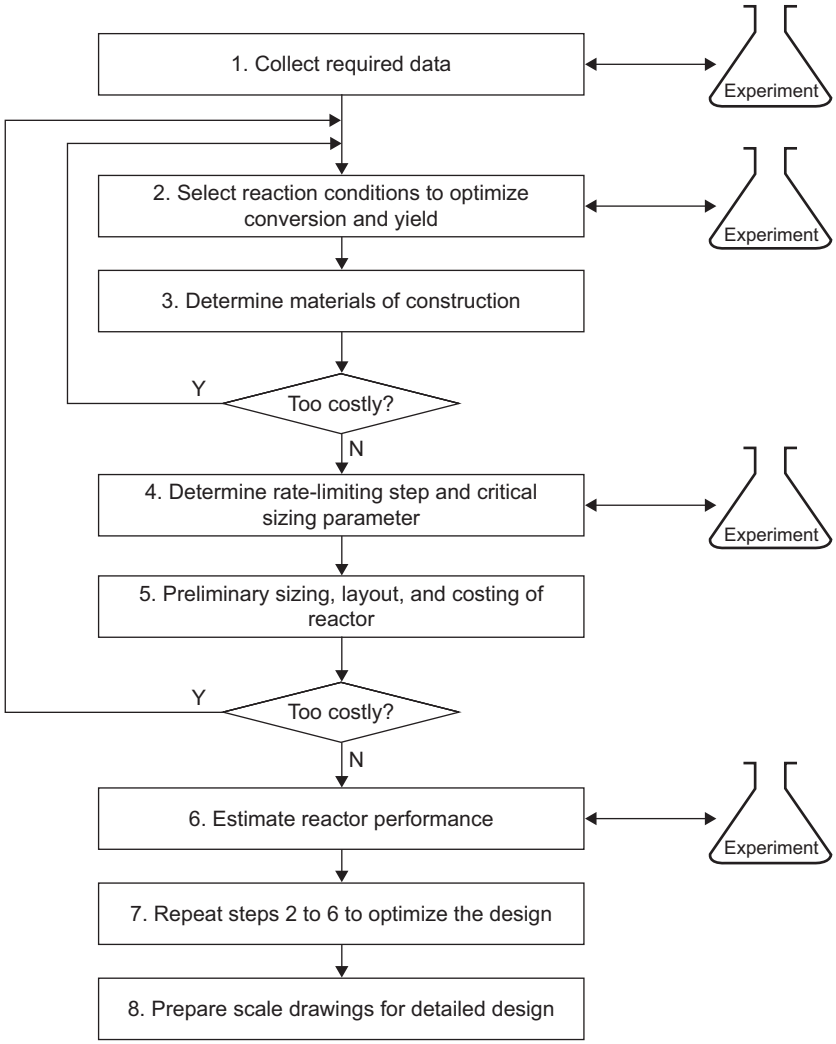


FIG. 15.1 General procedure for reactor design.

Step 1: Collect required data

Reactor design always requires more experimental input than the design of other process equipment. Some required parameters, such as heats of reaction and phase equilibrium constants, can be estimated using commercial process simulation models, while some parameters, such as diffusion coefficients and heat and mass transfer coefficients, can be predicted using correlations from the literature; however, almost all reaction rate constants must be measured experimentally.

Sources of reaction engineering data and methods for predicting heats of reaction and transport properties are given in Section 15.3.

The collection of reaction engineering data is often an iterative process. As the designer and researchers gain more insight into reactor performance, they may decide to operate the reactor under different conditions or may become aware of different by-products or feed contaminants that affect reaction rates. It is unlikely that the initial experiments or literature search will provide comprehensive information that covers all possible reaction conditions. It will thus be necessary to return to the laboratory and collect more data in the new region of interest at subsequent stages in the reactor design.

Step 2: Select reaction conditions

The reaction conditions should be chosen to optimize the reactor conversion, selectivity, and yield, within a reasonable reactor cost and allowing for a safe and controllable reactor design. The choice of reactor conditions is probably the most critical step in reactor design. Some of the conditions, such as the presence of contaminants in recycle streams, may be determined by other process considerations. The selection of reaction conditions is discussed in more detail in Section 15.4. The selection of reaction conditions will often govern the selection of reactor type. For example, if the reaction conditions cause all the reagents and products to be in the vapor phase, a stirred tank reactor will not be applicable.

Step 3: Determine materials of construction

When the reaction conditions have been specified, the designer can make a preliminary analysis of the materials of construction for the reactor. If the temperature, the pressure, or the presence of a particular component indicates that the reactor will need to be made from a costly alloy, the designer may be tempted to go back to the research team and try to identify a new set of reactor conditions. The selection of materials of construction is discussed in Chapter 6.

Step 4: Determine the rate limiting step and critical sizing parameters of the reactor

In this step the skills and knowledge of reaction engineering are deployed in elucidating the key parameters that determine the extent of reaction under the conditions previously specified. An experimental plan must be carried out under a broad enough range of conditions to determine what physical process limits the extent of reaction. In general, the reaction rate is usually limited by one of the following fundamental processes:

- Intrinsic kinetics: The rate of the reaction itself. In multistep reactions there will usually be one slowest step that governs the overall rate.
- Mass transfer rate: Mass transfer can be particularly important in multiphase reactions, where reagents must transfer between phases, and in reactions that use porous heterogeneous catalysts, where reagents and products must diffuse in and out of catalyst pores. Often, the measured rate of reaction will be confounded with the rate of mass transfer, and careful experimentation will be needed to separate the two effects and determine which is rate limiting for scale-up.
- Heat transfer rate: If a reaction is endothermic, then the temperature of the reaction mixture will decrease unless heat is added. The rate of heat addition can become the governing parameter in reactor sizing, and the reaction may even need to be carried out in a heat transfer device such as a heat exchanger or fired heater. Heat transfer to and from reactors is discussed in more detail in Section 15.6.
- Feed addition rate: If the reaction is exothermic, is very rapid, or requires a very low concentration of one of the components for optimal yield, the designer may choose to "starve" the reaction by limiting the feed rate of one of the reagents. Starving a reaction can be a good reactor control strategy for smaller reactors, but can be difficult to accomplish in larger reactors where uniform mixing is more difficult.
- Mixing rate: For very fast reactions, the time taken to mix the reagents can be the limiting step. If the reaction yield is sensitive to feed concentrations, the rate of mixing must be fast enough to ensure that the desired concentration

is achieved before reaction occurs (i.e., the reactor must be designed so that mixing is no longer rate limiting). Mixing is discussed in more detail in Section 15.5.

The rate-limiting step can be determined experimentally by collecting rate data and fitting a suitable model of reaction kinetics; see any of the references in the bibliography at the end of this chapter. Once the rate-limiting step has been determined, the designer will be able to specify a critical sizing parameter for the reactor. This will usually be one of the parameters given in Table 15.1. These parameters allow the reactor volume, volume or mass of catalyst, or contacting area for mass transfer to be scaled up relative to the mass or volumetric flow of reactor feed. The most common case that does not have a simple scaling parameter is when an endothermic reaction is limited by the rate of heat addition, which is discussed in more detail in Section 15.6.

The rate-limiting step can depend on the type of reactor that is selected for the experimental program. Care must be used when scaling up data to ensure that the same fundamental process will be rate limiting in a larger vessel.

TABLE 15.1 Reactor sizing parameters

Sizing parameter	Definition	Units	Comments
Residence time	$= \frac{\text{reactor volume}}{\text{volumetric flow rate}}$	Time	Most widely used reactor sizing parameter. Mainly used for homogeneously catalyzed reactions. Note that for liquid-phase reactions reactor volume refers to volume occupied by liquid, not total reactor volume. Volumetric flow rate should be calculated under average reactor conditions, which can be difficult for compressible gases if there is a significant change in temperature along the reactor.
Space velocity (also GHSV = gas hourly space velocity, LHSV = liquid hourly space velocity)	$= \frac{\text{volumetric flow rate}}{\text{reactor (or more often catalyst) volume}}$	Time^{-1} (usually by convention hr^{-1})	Usually used for reactors that employ solid catalysts. Volume usually refers to volume occupied by packed bed of catalyst, regardless of whether catalyst bed is expanded under process conditions. Volumetric flow rate should be calculated under average reactor conditions as noted above.
Weight or mass space velocity (WHSV = weight hourly space velocity)	$= \frac{\text{mass flow rate}}{\text{mass of catalyst}}$	Time^{-1} (usually by convention hr^{-1})	Usually used for reactors that employ solid catalysts. Use of WHSV avoids complications of allowing for changes in volumetric flow rate along reactor and variations in catalyst bed loading density between small laboratory reactors and full-scale reactors.
Number of transfer units	See Section 17.14.2. The definition is always a path integral of the inverse of concentration or partial pressure driving force. Different definitions can be used for vapor or liquid phase.	Dimensionless	Used for reactors where mass transfer between vapor and liquid phases is the rate-controlling step. See Section 17.14.2 for design of mass transfer contacting devices and Section 15.8 for more on multiphase reactors. Must be used with the appropriate definition of height of a transfer unit, which always includes the molar flow rate of one of the phases.

Step 5: Preliminary sizing, layout, and costing of reactor

Once the sizing parameter of the reactor has been obtained, the designer can estimate the reactor volume, catalyst volume, etc., that will be required at the design rate. The volume estimated is only the active reacting volume, and the reactor layout must also consider the following factors that may add to the volume required for the reactor vessel:

- Additional space needed for any internal heat transfer devices such as coils, stab-in bundles, quench zones, etc. (see Section 15.6).
- Additional space needed for vapor–liquid distribution, spargers, vapor–liquid segregation or redistribution (see Section 15.7).
- For liquid-phase stirred tank reactors, some inert vapor space should always be allowed so that the vessel is not filled with liquid. This makes pressure control much easier and reduces the possibility of hydraulic overpressure due to minor changes in flow during operation. A stirred tank reactor should not be designed to operate more

than 90% filled, and 65% to 75% is a better design guideline. If foaming can occur, then the level should be at the lower end of the range to allow space for a foam breaker.
- For packed or moving beds, space needed for inert catalyst support materials or support grids.
- For fluidized beds, space needed for fluid distribution grids, fluid−solid segregation, cyclones, transfer lines, allowance for bubble volume, etc. (see Section 15.7.3).

Other factors that can affect the overall reactor volume are discussed in Sections 15.6 to 15.10. Specific sizing guidelines are given for different reactor layouts in these sections.

The geometry of the reactor will depend on the desired flow pattern and mixing requirements. For simple reactors, the designer will select a vessel design that approximates one of the ideal mixing patterns described in Section 15.2.2. For more complex designs that involve several reaction zones, the designer will seek a geometry that arranges the different zones in the correct sequence, preferably (but not necessarily) within the same vessel. See Section 15.11.2 for more discussion of complex reactor networks. In some cases, the requirements of the reaction will dictate that a particular piece of equipment should be used. For example, if the reaction leads to precipitation of a product, it might be logical to use a crystallizer as the reactor, or if the reaction is endothermic and must be carried out at high temperature, then it may make sense to use a fired heater as the reactor.

Most reactors fall under the definition of pressure vessels, so once the length and diameter of the reactor have been selected, the wall thickness can be found using the methods described in Chapter 14. The cost of the reactor can then be built up from the cost of the pressure vessel plus the cost of the internals listed earlier. Methods for estimating capital costs for equipment components are given in Section 7.5. The sizing and costing of reactors are illustrated in Examples 15.4, 15.5, and 15.6.

If the preliminary reactor design is too costly, the designer should revisit Step 2 and see if other conditions can be found that will lead to an improved design.

Step 6: Estimate reactor performance

It is important to confirm that the reactor design will actually achieve the target conversion and selectivities for main products and by-products. Unfortunately, it is often impossible to be fully satisfied without building and testing a full-scale reactor, which is a very expensive proposition.

Historically, chemical companies would go through multiple steps of pilot plant scale-up to validate their reactor designs. Successive pilot plants would be built with the scale of production increasing by one or two orders of magnitude each time. This gradual approach to scale-up was expensive and delayed the market launch of new products and process technologies.

Nowadays, a more common approach is to use a combination of experimental methods and computer modeling to attempt to predict the full-scale performance. This allows the design team to eliminate some of the intermediate steps in scale-up and go from well-designed small pilot plants to a demonstration unit that may be approaching full scale in a single step. Computer simulation methods for reactor analysis are discussed in Section 15.11, and methods for determining actual reactor performance are described in Section 15.12.

Step 7: Optimize the design

If necessary, Steps 2 to 6 can be repeated to optimize the design. Optimization to reduce the reactor cost is usually a waste of time because the cost of the reactor is typically a relatively small fraction of the total capital cost; however, if the reactor validation experiments showed the presence of unexpected components or showed different selectivities than were found at smaller scale, it will be necessary to reevaluate the overall process optimization and confirm that the target conversion, yields, and selectivities still apply.

Step 8: Prepare scale drawings for detailed design

The final step for the chemical engineer is to make an effective hand-off of the design to the specialized mechanical engineering designer or design team. Because most reactors require substantial internals and ancillary equipment such as agitators, heat transfer coils, etc., the mechanical design of the vessel is rarely trivial. The mechanical engineer needs a complete specification of the vessel and internals, so as to be able to make detailed designs of nozzles, reinforcing rings, internal and external support brackets, and other features. The best means for transmitting all of the required specifications is usually for the reactor designer and the mechanical designer to collaborate on producing scale drawings that show all of the necessary features. Often the mechanical engineer will be involved throughout the design process and will already have a good understanding of the reactor requirements.

15.2.2 Ideal and real reactors

It is convenient to describe reactors in terms of how closely they approximate the behavior of the two extreme types of ideal reactor: the plug flow reactor (PFR) and the well-mixed reactor (WMR). In fact, it can be shown that real reactors can be modeled as networks or combinations of multiple plug flow and well-mixed reactors; see Section 15.11.2.

Plug-flow reactor (PFR)

In perfect plug flow, each batch of material that enters the reactor moves through the reactor together, mixing and reacting only with material that entered at the same time, and all leave the reactor together. In a PFR with tubular geometry, there is perfect radial mixing but no axial mixing. All material that flows through the reactor has exactly the same residence time, τ, and all material experiences the same profile of temperature and concentration as it moves along the reactor. A perfectly mixed batch reactor behaves the same as a PFR, with the material moving through time instead of space.

A PFR can be sized by considering an incremental slice of the reactor, as shown in Fig. 15.2. The change in molar flow rate of a reacting component (usually a feed component) due to the reaction is equal to the rate of reaction in the increment:

$$\mathrm{d}M = \Re \mathrm{d}V \tag{15.1}$$

where

M = molar flow rate = volume flow rate × molar concentration
$\mathrm{d}V$ = incremental volume
$\Re$ is an expression for the rate of reaction per unit volume

Because both the rate of reaction and the molar flow rate can be written in terms of the concentration or partial pressure of the reacting components, Equation 15.1 can be integrated along the reactor length to give a relationship between reactor residence time and concentration or conversion. Different relationships are obtained depending on the form of expression for the rate of reaction; see any of the books cited in the bibliography at the end of this chapter for multiple solved examples.

Well-mixed reactor (WMR)

In a perfect WMR, the entire contents of the vessel are at the same temperature and concentration and there is no spatial variation in any mixture property. The fluid leaving the WMR is therefore at the same concentration and temperature as the vessel contents. Material entering the WMR is immediately mixed with the contents and comes to the same conditions. Some of the material that enters can leave immediately, whereas some leaves much later, so there is a broad distribution in residence time, as shown in Fig. 15.3.

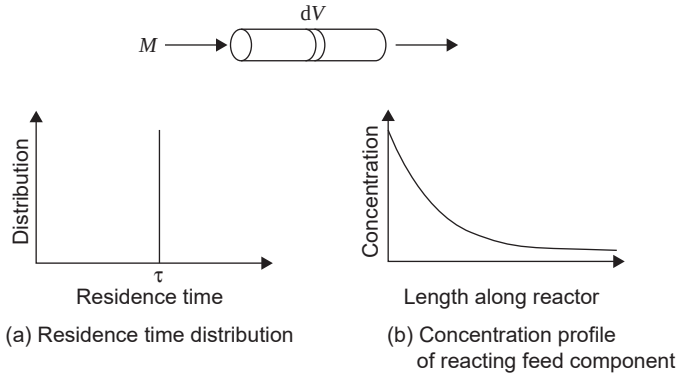


FIG. 15.2 Plug-flow reactor.

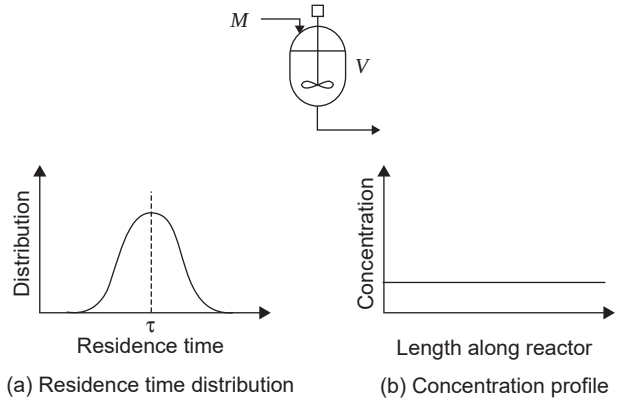


FIG. 15.3 Well-mixed reactor.

A WMR can be sized by solving a material balance across the reactor:

$$M_{in} - M_{out} = \Re V \tag{15.2}$$

where

M_{in} = molar flow rate of any component into the reactor
M_{out} = molar flow rate of any component out of the reactor
V = reactor volume

As with the PFR, the molar flow rate can be expressed in terms of volume flow and concentration, and the rate of reaction can also be written in terms of concentrations, allowing Equation 15.2 to be restated as a relationship between residence time and concentration or conversion. The books cited in the bibliography provide examples of different expressions obtained with different reaction rate equations.

Real reactors

Few real reactors achieve ideal reactor performance, although many reactors are close enough that ideal reactor performance can be assumed for modeling purposes; see Section 15.11. Some real reactor types that have performance close to that of ideal reactors are shown in Fig. 15.4.

Near plug flow conditions can be obtained in tubular or serpentine reactors, but allowance must be made for some degree of axial dispersion. Simple tubular (pipeline) reactors are normally used for homogeneous gas-phase reactions, for example, in the thermal cracking of petroleum crude oil fractions to ethylene and the thermal decomposition of dichloroethane to vinyl chloride. Tubular reactors can also be used for homogeneous liquid-phase reactions. Single-phase flow through packed beds or heat exchanger or furnace tubes is a good approximation of plug flow, as is the flow in a transport-phase fluidized bed. It is not necessary for a reactor to be long and thin to be in plug flow. A thin bed of catalyst is often loaded into a radial-flow reactor, in which the fluid flows radially through a bed of catalyst retained between perforated screens (see Section 15.7.3 and Fig. 15.29). Although the path length through the bed is short, there is little opportunity for back-mixing, and plug flow is a good approximation.

Continuous stirred tank reactors often provide a reasonable approximation of WMR performance, although mixing is never perfect. The effect of poor mixing is usually to skew the residence time distribution, giving a longer tail to the distribution. Sparged tanks and lift-tube reactors are well-mixed in the liquid phase, although plug flow with respect to the vapor phase. A fluidized bed operated in bubbling-bed mode is well-mixed with respect to the solids and can be either well-mixed or plug flow with respect to the liquid or vapor that is causing fluidization; see Section 15.7.3.

Examples of real reactors will be introduced in the following sections, particularly in Sections 15.5 to 15.10. The use of networks of ideal reactors to model real reactor performance is discussed in Section 15.11.2. The volumes by Rase (1977, 1990) cover the practical aspects of reactor design and include case studies of industrial reactors. Henkel (2005) catalogs different types of industrial reactors and gives examples of the types of reaction carried out in each.

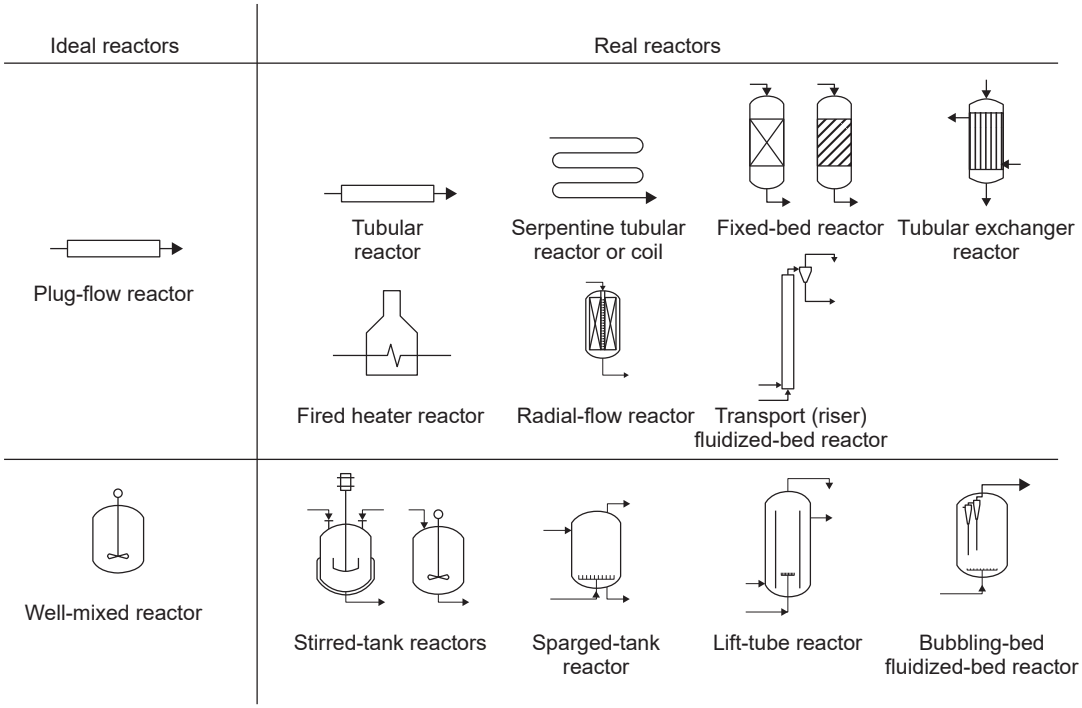


FIG. 15.4 Ideal reactors and some real reactors that approximate the same flow pattern.

15.3 Sources of reaction engineering data

This section provides a brief overview of sources of reaction engineering data such as enthalpy and Gibbs free energy of reaction, equilibrium constants, reaction rate constants, activation energies, and mass transfer properties.

15.3.1 Enthalpy of reaction

The amount of heat given out in a chemical reaction depends on the conditions under which the reaction is carried out. The standard heat of reaction is the heat released when the reaction is carried out under standard conditions: pure components, pressure 1 atm (1.01325 bar), and temperature usually, but not necessarily, 25 °C. Care must be taken to correct the heat of reaction to the temperature and pressure of the process.

Values for the standard heats of reaction for the reactions used in the production of commercial chemicals can usually be found in the literature or can be calculated from heats of formation or combustion. A useful source of data on heats of formation and combustion is the critical review of the literature by Domalski (1972).

Benson developed a detailed group contribution method for the estimation of heats of formation; see Benson (1976) and Benson et al. (1969). He estimated the accuracy of the method to be from ±2.0 kJ/mol for simple compounds to about ±12 kJ/mol for highly substituted compounds. Benson's method and other group contribution methods for the estimation of heats of formation are described by Reid et al. (1987). Group contribution approaches are used by commercial process simulation programs to estimate enthalpies of formation for user-specified compounds if the user does not manually enter a heat of formation. Group contribution approaches are also sometimes used for library compounds.

When quoting heats of reaction, the basis should be clearly stated, either by giving the chemical equation, for example:

$$NO + \frac{1}{2}O_2 \rightarrow NO_2 \quad \Delta H_r^\circ = -56.68 \text{ kJ}$$

(the equation implies that the quantity of reactants and products are moles), or by stating to which quantity the quoted value applies:

$$\Delta H_r^\circ = -56.68 \text{ kJ per mol } NO_2$$

The reaction is exothermic, and the enthalpy change ΔH_r° is therefore *negative*. The heat of reaction $-\Delta H_r^\circ$ is *positive*. The superscript ° denotes a value at *standard* conditions, and the subscript *r* implies that a chemical reaction is involved.

The state of the reactants and products (gas, liquid, or solid) should also be given if the reaction conditions are such that they may exist in more than one state; for example:

$$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(g), \quad \Delta H_r^\circ = -241.6 \text{ kJ}$$

$$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l), \quad \Delta H_r^\circ = -285.6 \text{ kJ}$$

The difference between the two heats of reaction is the latent heat of the water formed.

In process design calculations, it is usually more convenient to express the heat of reaction in terms of the moles of product produced for the conditions under which the reaction is carried out, kJ/mol product.

Effect of temperature on heat of reaction

The heat of reaction must be estimated at process conditions for use in reactor design. Failure to correct the heat of reaction can lead to gross overestimates of the required heating or cooling duty.

Standard heats of reaction can be converted to other reaction temperatures by making a heat balance over a hypothetical process, in which the reactants are brought to the standard temperature, the reaction carried out, and the products then brought to the required reaction temperature, as illustrated in Fig. 15.5.

$$\Delta H_{r,T} = \Delta H_r^\circ + \Delta H_{prod} + \Delta H_{react} \tag{15.3}$$

where :

$-\Delta H_{rT}$ = heat of reaction at temperature T

$\Delta H_{\text{react.}}$ = enthalpy change to bring reactants to standard temperature (which will be negative, as the reagents are being cooled)

$\Delta H_{\text{prod.}}$ = enthalpy change to bring products to reaction temperature, T

Effect of pressure on heat of reaction

Equation 15.3 can be written in a more general form:

$$\Delta H_{r,P,T} = \Delta H_r^\circ + \int_1^P \left[\left(\frac{\partial H_{\text{prod.}}}{\partial P} \right)_T - \left(\frac{\partial H_{\text{react.}}}{\partial P} \right)_T \right] dP + \int_{298}^T \left[\left(\frac{\partial H_{\text{prod.}}}{\partial T} \right)_P - \left(\frac{\partial H_{\text{react.}}}{\partial T} \right)_P \right] dT \tag{15.4}$$

Where: P = pressure

If the effect of pressure is likely to be significant, the change in enthalpy of the products and reactants, from the standard conditions, can be evaluated to include both the effects of temperature and pressure (for example, by using tabulated values of enthalpy) and the correction made in a similar way to that for temperature only.

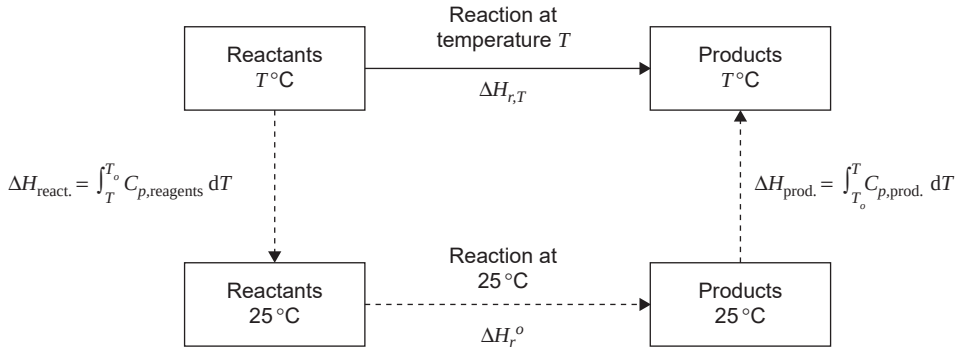


FIG. 15.5 ΔHr at temperature T.

Estimation of heat of reaction using process simulation programs

Commercial process simulation programs can easily be manipulated to give quick estimates of reactor heating or cooling duty at process temperature and pressure. For most library compounds, the heat of reaction will be calculated using tabulated heats of formation and heat capacities that have been measured experimentally, but for user-specified compounds and possibly some library compounds, group contribution methods will be used to estimate the heat of formation and heat capacity, and so there will be more uncertainty in the answer.

When literature data on standard heat of reaction are available, a quick check of the process simulation software can be made by simulating an isothermal reactor at 25 °C. The heating or cooling duty calculated should match the standard heat of reaction.

Simulation programs are particularly helpful when several reactions are occurring at the same time, in which case calculating the overall reactor duty manually becomes tedious.

When using simulation programs to estimate reactor heating or cooling requirements, the following points should be kept in mind:

- Make sure the feeds to the reactor in the simulation model are at the temperature and pressure that the real feeds will be at. If a feed is hotter or colder than the reaction temperature, the change in sensible heat can have a significant effect on the reactor heat balance.
- Be sure to include all reactions that have a significant extent of reaction or conversion. It is best to use a conversion or yield reactor when predicting reactor heating or cooling duty unless the process gives products at equilibrium. See Section 4.5.1 for a discussion of different standard reactor models.
- To estimate the heating or cooling requirement, provide a heat stream into the reactor. Do not specify the duty of this heat stream. Instead, specify the desired temperature of the reactor products; the simulator will then calculate the required heating or cooling duty.

The heating or cooling duty predicted from a simulation model should be benchmarked against experimental data whenever possible. It may be difficult to accurately measure heat of reaction in a small pilot plant, and allowance for additional heating or cooling above that predicted by the simulation should be made during scale-up.

Example 15.1

This example illustrates the manual calculation of a reactor heat balance.

Vinyl chloride (VC) is manufactured by the pyrolysis of 1,2-dichloroethane (DCE). The reaction is endothermic. The flow rates to produce 5000 kg/h at 55% conversion are shown in Fig. 15.6.

The reactor is a pipe reactor heated with fuel gas, gross calorific value 33.5 MJ/m^3. Estimate the quantity of fuel gas required.

Solution

$$\text{Reaction: } C_2H_4Cl_2(g) \rightarrow C_2H_3Cl(g) + HCl(g) \quad \Delta H_r^\circ = 70{,}224 \text{ kJ/kmol}$$

The small quantity of impurities, less than 1%, that would be present in the feed has been neglected for the purposes of this example. Also, the selectivity for VC has been taken as 100%. It would be in the region of 99% at 55% conversion.

Heat capacity data, for vapor phase:

$$C_p^\circ = a + bT + cT^2 + dT^3 \text{ kJ/kmolK}$$

	a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$
VC	5.94	20.16	−15.34	47.65
HCl	30.28	−0.761	1.325	−4.305
DCE	20.45	23.07	−14.36	33.83

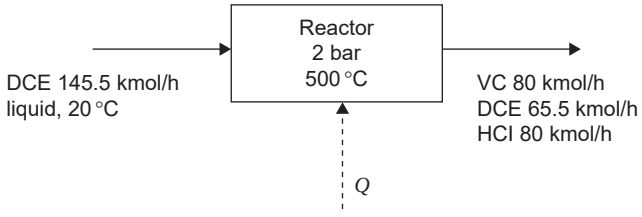


FIG. 15.6 Vinyl chloride reactor example.

for liquid phase: DCE at 20 °C, $C_p = 116$ kJ/kmol K, taken as constant over a temperature rise from 20 to 25 °C.
Latent heat of vaporization of DCE at 25 °C = 34.3 MJ/kmol.

At 2 bar pressure, the change in C_p with pressure will be small and will be neglected. Take base temperature as 25 °C (298 K), the standard state for ΔH_r°.

$$\text{Enthalpy of feed} = 145.5 \times 116(293-298) = -84{,}390 \text{ J/h} = \underline{\underline{-84.4 \text{ MJ/h}}}$$

$$\text{Enthalpy of product stream} = \int_{298}^{773} \sum (n_i C_p)\, dT$$

Component	n_i (mol/h)	$n_i a$	$n_i b \times 10^2$	$n_i c \times 10^5$	$n_i d \times 10^9$
VC	80	475.2	1612.8	−1227.2	3812.0
HCl	80	2422.4	−60.88	106.0	−344.4
DCE	65.5	1339.5	1511.0	−940.6	2215.9
$\sum n_i C_p$		4237.1	3063.0	−2061.8	5683.5

$$\int_{298}^{773} n_i C_p \, dT = \int_{298}^{773} \left(4237.1 + 3063.0 \times 10^{-2} T - 2061.8 \times 10^{-5} T^2 + 5683.5 \times 10^{-9} T^3\right) dT$$
$$= 7307.3 \text{ MJ/h}$$

Heat consumed in system by the endothermic reaction = $\Delta H_r^\circ \times$ moles produced

$$= 70{,}224 \times 80 = 5{,}617{,}920 \text{ kJ/h} = \underline{\underline{5617.9 \text{ MJ/h}}}$$

Heat to vaporize feed (gas phase reaction)

$$= 34.3 \times 145.5 = \underline{\underline{4990.7 \text{ MJ/h}}}$$

Heat balance:

$$\text{Output} = \text{Input} + \text{Consumed} + \text{Q}$$
$$\text{Q} = H_{\text{product}} - H_{\text{feed}} + \text{Consumed}$$
$$= 7307.3 - (-84.4) + (5617.9 + 4990.7) = \underline{\underline{18{,}002.3 \text{ MJ/h}}}$$

Taking the overall efficiency of the furnace as 70%, the gas rate required:

$$= \frac{\text{Heat input}}{(\text{calorific value} \times \text{efficiency})}$$
$$= \frac{18{,}002.3}{33.5 \times 0.7} = \underline{\underline{768 \text{ m}^3/\text{h}}}$$

15.3.2 Equilibrium constant and Gibbs free energy

The reaction equilibrium constant is related to the change in Gibbs free energy of reaction by the equation:

$$\Delta G = -RT \ln K \tag{15.5}$$

where:

$-\Delta G$ = change in Gibbs free energy as a result of reaction at temperature T
R = ideal gas constant
K = reaction equilibrium constant, defined as:

$$K = \prod_{i=1}^{n} a_i^{\alpha_i} \tag{15.6}$$

where:

a_i = activity of component i
α_j = stoichiometric coefficient of component i, defined such that stoichiometric coefficients are positive for products and negative for reagents (so reagents end up on the denominator)
n = total number of components

Equilibrium constants for many commercial process reactions can be found in the literature using academic search tools such as the ACS chemical abstracts tool *SciFinder*.

The equilibrium constant is useful for understanding the equilibrium of the main process reaction and for assuring thermodynamic consistency between the rates of forward and reverse reactions; but when there are several simultaneous reactions, the equilibrium concentration is more easily evaluated by minimizing Gibbs free energy. This is the method used in the Gibbs reactor model that is found in all commercial process simulation programs. The use of Gibbs reactors and equilibrium reactors in process simulation is discussed in Section 4.5.1.

Many of the comments made about the enthalpy of reaction also apply to the Gibbs energy of reaction and by extension to the estimation of equilibrium constants. Care must be taken to correct the Gibbs energy to the process conditions, and the equations for variation of Gibbs energy and equilibrium constant with temperature and pressure can be found in most reaction engineering or thermodynamics textbooks. When using a process simulation program to estimate equilibrium constants (or equilibrium composition), the designer should be aware that the program may be using group contribution methods to estimate Gibbs energies and heat capacities, thereby introducing a higher margin of error into the result.

The measurement of actual chemical equilibrium is often more complex than might be expected. In principle, a reaction system that is held at the same conditions for a long enough time will reach equilibrium, allowing the equilibrium composition to be measured. In practice, this can be difficult because of the following factors:

- In real reacting systems, often many components are present, and it may be difficult to determine which species are able to react with each other and contribute to the overall equilibrium. This is particularly problematic for processes that involve electrolyte solutions (including most biological processes) and processes that deal with high-molecular-weight hydrocarbon compounds. It may not be practical to carry out enough experiments to determine all of the possible equilibrium constants.
- If the composition is not measured *in situ* in the reaction mixture, reactions may occur during sample withdrawal, preparation, and analysis, leading to a false estimate of composition. This is a significant problem for high-temperature reactions, as the sample will typically become cooled as it is withdrawn for analysis, and so the composition that is measured may have moved away from the high-temperature equilibrium composition. Rapid sample quench methods can improve accuracy, but for some very fast reactions, there will still be an offset.
- Slow reactions, such as thermal degradation, may affect the ultimate equilibrium, but may or may not be important for process purposes.

When using equilibrium constants from the literature, the design engineer should pay careful attention to the experimental design and test methodology to be satisfied that the values reported are consistent with the conditions of the test reactor.

15.3.3 Reaction mechanisms, rate equations, and rate constants

One of the most difficult concepts in reaction engineering for novice engineers to grasp is that you don't need to know the reaction rate to make a preliminary design of a reactor. If the required residence time or space velocity has been determined experimentally, the reactor design can be completed and scaled up without requiring any knowledge of the kinetics. In the context of industrial process development, it is usually necessary to complete a preliminary reactor design and process economic evaluation long before sufficient data have been collected to fit a predictive model of all the reactions involved.

The reaction rate equation expresses the rate of removal of a reagent or formation of a product, usually as a function of the concentrations of components present in the mixture, temperature, pressure, and other properties such as adsorption equilibrium and mass transfer properties. Few reactions of industrial significance have simple first- or second-order rate equations, for the following reasons:

- Most industrial processes use heterogeneous catalysis or enzymes, leading to Langmuir–Hinshelwood–Hougen–Watson or Michaelis–Menten kinetics.
- Many industrial reactions require mass transfer between vapor and liquid or between two liquid phases, leading to overall rate expressions that are modified to include mass transfer effects.

- Many industrial reactions have multistep mechanisms, leading to rate expressions that do not necessarily follow the overall reaction stoichiometry.
- In most industrial processes there are several competing side reactions in addition to the main reaction. The rate of feed consumption or product removal is then the sum of contributions from each of these reactions.

Having said this, in many cases, the main process reaction can be approximated as first or second order over a narrow range of temperature, pressure, and concentration for purposes of estimating the required residence time to achieve a given conversion.

Reaction rate equations and rate constants cannot reliably be predicted from first principles and must be determined by fitting to experimental data. The books listed in the bibliography at the end of this chapter give details of how to measure rate constants experimentally; see also Green and Southard (2018). Stewart and Caracotsios (2008) provide an excellent introduction to techniques for model discrimination and parameter estimation.

The chemical engineering literature contains an abundance of papers that report reaction mechanisms and rate equations. These can be located through the ACS Chemical Abstract Service using *SciFinder*. Before using kinetics data from the literature, the designer should make a careful search for other papers that confirm the results, and if possible, should validate the rate model against commercial or pilot plant data.

Reaction mechanisms can be very sensitive to process or experimental conditions, and the rate-limiting step may change as a result of relatively small changes in temperature or concentrations, particularly for solid-catalyzed reactions. Rate equations are always a fit of experimental or plant data and should only be used for interpolation within the range of conditions spanned by the data. If extrapolation is necessary, more data must be collected to confirm that the rate model still applies. This is particularly important for exothermic reactions, which have the potential to suffer runaway. The mechanism and kinetics of exothermic reactions should always be studied over a wide enough range of temperature to allow safe design of the reactor system and collect necessary data for venting and relief load calculations; see Section 15.13.3.

15.3.4 Transport properties

Heat transfer

Heat transfer coefficients are needed for the design of internal heating or cooling devices and for reactions that are carried out in fired heaters or heat exchangers. Heat transfer coefficients can be predicted using the methods given in Chapter 19 for tubular exchangers, fired heaters, internal coils, jacketed vessels, and stirred tanks.

When catalyst is packed inside the tubes of a heat exchanger, the internal heat transfer coefficient is increased. The tube-side heat transfer coefficient for a tube packed with pellets can be estimated from the correlations of Leva (1949).

$$\text{For heating:}\ \frac{h_i d_t}{\lambda_f} = 0.813\left(\frac{\rho_f\, u\, d_p}{\mu}\right)^{0.9} e^{-6d_p/d_t} \tag{15.7}$$

$$\text{and for cooling:}\ \frac{h_i d_t}{\lambda_f} = 3.50\left(\frac{\rho_f\, u\, d_p}{\mu}\right)^{0.7} e^{-4.6d_p/d_t} \tag{15.8}$$

Where:

h_i = tube-side heat transfer coefficient for a packed tube
d_t = tube diameter
λ_f = fluid thermal conductivity
ρ_f = fluid density
u = superficial velocity
d_p = effective particle diameter
μ = fluid viscosity

Diffusivities

Diffusion coefficients are needed in the design of catalytic reactions where mass transfer can limit the rate of reaction, as well as in mass transfer processes, such as gas absorption, distillation, and liquid–liquid extraction. Experimental values for some common systems can be found in the literature, but for most design work, the values must be estimated.

For gases, the equation developed by Fuller et al. (1966) is easy to apply and gives reliable estimates:

$$D_v = \frac{1.013 \times 10^{-7} T^{1.75} \left(\frac{1}{M_a} + \frac{1}{M_b}\right)^{1/2}}{P\left[\left(\sum_a v_i\right)^{1/3} + \left(\sum_b v_i\right)^{1/3}\right]^2} \tag{15.9}$$

where:

D_v = diffusivity, m^2/s
T = temperature, K
M_a, M_b = molecular masses of components a and b
P = total pressure, bar
$\sum_a v_i$, $\sum_b v_i$ = the summation of the special diffusion volume coefficients for components a and b, given in Table 15.2

Fuller's method is illustrated in Example 15.2.

The diffusivity of components in the liquid phase can be predicted using the equation developed by Wilke and Chang (1955), given here.

$$D_L = \frac{1.173 \times 10^{-13} (\phi M_w)^{0.5} T}{\mu V_m^{0.6}} \tag{15.10}$$

where D_L = liquid diffusivity, m^2/s.
Φ = an association factor for the solvent.
= 2.6 for water (some workers recommend 2.26).
= 1.9 for methanol.
= 1.5 for ethanol.
= 1.0 for unassociated solvents.
M_w = molecular mass of solvent.
μ = viscosity of solvent, mN s/m^2.
T = temperature, K.
V_m = molar volume of the solute at its boiling point, m^3/kmol. This can be estimated from the group contributions given in Table 15.3.

TABLE 15.2 Special atomic diffusion volumes

Atomic and structural diffusion volume increments			
C	16.5	Cl	19.5*
H	1.98	S	17.0*
O	5.48	Aromatic or hetrocyclic rings	−20.0
N	5.69*		
Diffusion volumes of simple molecules			
H_2	7.07	CO	18.9
D_2	6.70	CO_2	26.9
He	2.88	N_2O	35.9
N_2	17.9	NH_3	14.9
O_2	16.6	H_2O	12.7
Air	20.1	CCL_2F_2	114.8*
Ne	5.59	SF_6	69.7*
Ar	16.1	Cl_2	37.7*
Kr	22.8	Br_2	67.2*
Xe	37.9*	SO_2	41.1*

*Value based on only a few data points.
From Fuller et al. (1966).

TABLE 15.3 Structural contributions to molar volumes, m^3/kmol

Molecular volumes							
Air	0.0299	CO_2	0.0340	H_2S	0.0329	NO	0.0236
Br_2	0.0532	COS	0.0515	I_2	0.0715	N_2O	0.0364
Cl_2	0.0484	H_2	0.0143	N_2	0.0312	O_2	0.0256
CO	0.0307	H_2O	0.0189	NH_3	0.0258	SO_2	0.0448
Atomic volumes							
As	0.0305	F	0.0087	P	0.0270	Sn	0.0423
Bi	0.0480	Ge	0.0345	Pb	0.0480	Ti	0.0357
Br	0.0270	H	0.0037	S	0.0256	V	0.0320
C	0.0148	Hg	0.0190	Sb	0.0342	Zn	0.0204
Cr	0.0274	I	0.037	Si	0.0320		
Cl, terminal, as in RCl			0.0216	in higher esters, ethers		0.0110	
medial, as in R—CHCl—R			0.0246	in acids		0.0120	
Nitrogen, double-bonded			0.0156	in union with S, P, N		0.0083	
triply bonded, as in nitriles			0.0162	three-membered ring		−0.0060	
in primary amines, RNH_2			0.0105	four-membered ring		−0.0085	
in secondary amines, R_2NH			0.012	five-membered ring		−0.0115	
in tertiary amines, R_3N			0.0108	six-membered ring as in benzene, cyclohexane, pyridine		−0.0150	
Oxygen, except as noted below			0.0074				
in methyl esters			0.0091	Naphthalene ring		−0.0300	
in methyl ethers			0.0099	Anthracene ring		−0.0475	

From Gambill (1958).

The Wilke–Chang method is illustrated in Example 15.3.

The Wilke–Chang correlation is shown graphically in Fig. 15.7. This figure can be used to determine the association constant for a solvent from experimental values for D_L in the solvent.

The Wilke–Chang equation gives satisfactory predictions for the diffusivity of organic compounds in water, but not for water in organic solvents.

Example 15.2

Estimate the diffusivity of methanol in air at atmospheric pressure and 25 °C.

Solution

Diffusion volumes from Table 15.2; methanol:

Element	v_i		No. of	
C	16.50	×	1 =	16.50
H	1.98	×	4 =	7.92
O	5.48	×	1 =	5.48
			$\sum_a v_i$	29.90

Diffusion volume for air = 20.1

1 standard atmosphere = 1.013 bar

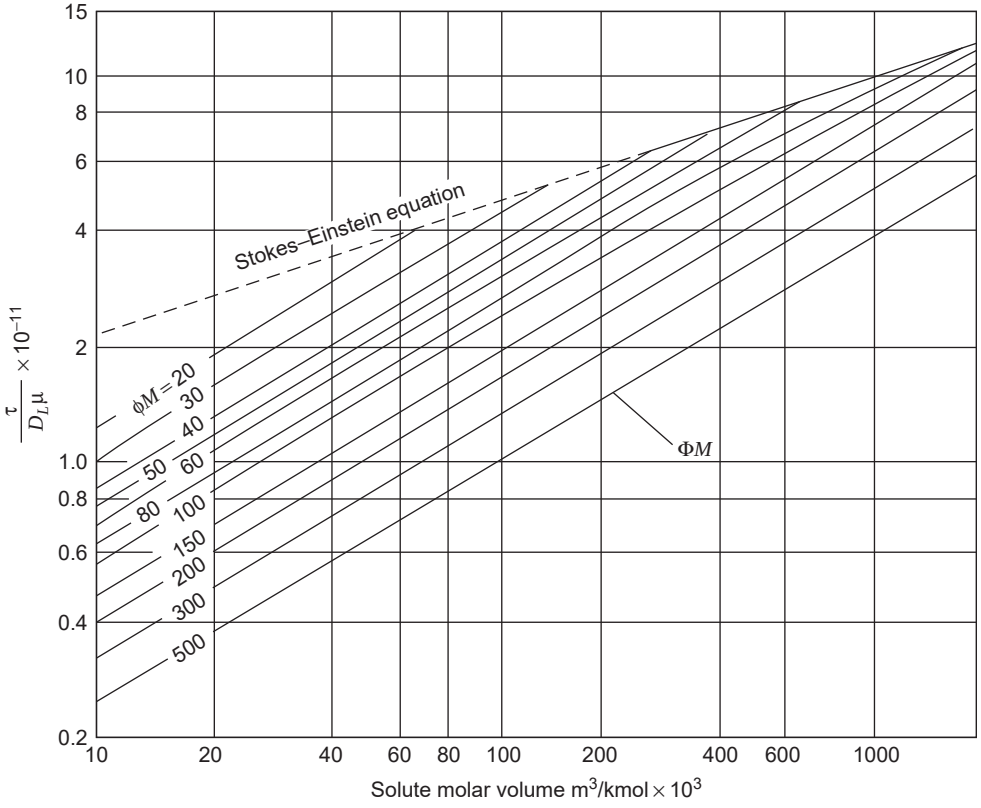


FIG. 15.7 The Wilke–Chang correlation.

molecular mass $CH_3OH = 32$, air $= 29$

$$D_v = \frac{1.013 \times 10^{-7} \times 298^{1.75}(1/32 + 1/29)^{1/2}}{1.013\left[(29.90)^{1/3} + (20.1)^{1/3}\right]^2} \tag{15.9}$$

$$= \underline{\underline{16.2 \times 10^{-6} \text{m}^2/\text{s}}}$$

Experimental value, 15.9×10^{-6} m^2/s

Example 15.3

Estimate the diffusivity of phenol in ethanol at 20 °C (293 K).

Solution

Viscosity of ethanol at 20 °C, 1.2 mNs/m^2
Molecular mass, 46
Molar volume of phenol, C_6H_5OH, from Table 15.3:

Atom	Vol.		No. of		
C	0.0148	×	6	=	0.0888
H	0.0037	×	6	=	0.0222
O	0.0074	×	1	=	0.0074
ring	−0.015	×	1	=	−0.015
					0.1034 m^3/k mol

$$D_L = \frac{1.173 \times 10^{-13}(1.5 \times 46)^{0.5} 293}{1.2 \times 0.1034^{0.6}} = \underline{\underline{9.28 \times 10^{-10}\ \text{m}^2/\text{s}}} \tag{15.10}$$

Experimental value, 8×10^{-10} m^2/s, error 16%.

Mass transfer coefficients

Mass transfer coefficients are used in multiphase reactors, for example, in calculating the flux of material to and from the surface of solid catalysts and in calculating the mass flux across a vapor–liquid interface. It is very unlikely that a suitable mass transfer coefficient for a given reactor design can be found in the literature, so the mass transfer coefficient must usually be estimated using correlations.

For a single pellet or droplet suspended in a fluid, the mass transfer coefficient can be predicted using the Frössling equation (Frössling, 1938):

$$\text{Sh} = 2.0 + 0.552\ \text{Re}^{0.5}\text{Sc}^{0.33} \tag{15.11}$$

where: Sh = Sherwood number = $k\ d_p\ /D$
k = mass transfer coefficient, m/s
d_p = particle diameter, m
D = diffusivity, m^2/s
Re = Reynolds number = $\rho_f\ u_p\ d_p\ /\mu_f$
u_p = particle velocity relative to the fluid, m/s
Sc = Schmidt number = $\mu_f\ /\rho_f\ D$

For mass transfer to a packed bed of particles, the equation of Gupta and Thodos (1963) can be used:

$$\text{Sh} = 2.06\frac{1}{\varepsilon}\text{Re}^{0.425}\text{Sc}^{0.33} \tag{15.12}$$

where: ε = bed void fraction

Re is calculated using the superficial velocity of the fluid through the bed

Mass transfer between vapor and liquid in packed beds is discussed in Section 17.14. Mass transfer from a falling drop to a vapor can be estimated using Frössling's equation, Equation 15.11. Mass transfer between vapor and liquid in an agitated vessel can be predicted using the equations given by Van't Riet (1979):

$$\text{For air} - \text{water}: k_L a = 0.026\left(\frac{P_a}{V_{liq}}\right)^{0.4} Q^{0.5} \tag{15.13}$$

$$\text{and for air} - \text{water} - \text{electrolyte}: k_L a = 0.002\left(\frac{P_a}{V_{liq}}\right)^{0.7} Q^{0.2} \tag{15.14}$$

where:

k_L = mass transfer coefficient, m/s
a = interfacial area per unit volume, m^2/m^3
Q = gas volumetric flow rate, m^3/s
V_{liq} = liquid volume, m^3
P_a = agitator power input, W

The mass transfer coefficient for other low-viscosity systems can be calculated from the air–water coefficient using the method suggested by Fair (1967):

$$\frac{(k_L a)_{system}}{(k_L a)_{air-water}} = \left(\frac{D_{L,system}}{D_{L,air-water}}\right)^{0.5} \tag{15.15}$$

where D_L = liquid phase diffusivity, m^2/s

Green and Southard (2018) recommend caution when using mass transfer correlations for vapor–liquid systems if surfactants may be present. Whenever possible, the results predicted from correlations should be benchmarked against pilot plant measurements.

15.4 Choice of reaction conditions

The choice of operating conditions for carrying out a reaction plays a large role in determining what type of reactor will be used. Although the best conditions will typically be determined experimentally by the research team, the reactor designer can guide the chemists to conditions that will lead to a more optimal overall design. Chemists are generally trained to optimize syntheses by maximizing the reactor yield of desired product; however, the conditions that maximize reactor yield will usually not be optimal from a process standpoint, as operation at lower feed conversion usually improves selectivity and hence overall process yield. By performing a preliminary economic analysis, as described in Section 2.6, the design engineer can set yield and selectivity targets that will focus the experimentation on conditions that are more likely to lead to an optimum overall process.

When the final reaction conditions have been selected, it is important to confirm experimentally that the target process yields and selectivities are obtainable in practice. The validation of reactor designs is discussed in Section 15.12.

15.4.1 Chemical or biochemical reaction

Biochemical reactions involve the use of microorganisms, cells, or enzymes to carry out the process chemistry. Many compounds can be made by both chemical and biochemical routes, but some highly valuable products can only be synthesized using biochemical techniques.

Biochemical reactions must be carried out under conditions that preserve the effectiveness of the biological agent: the microorganism, cells, or enzymes that carry out the reaction. Although life has evolved to exploit almost every condition encountered on our planet, most living systems are not robust to a wide variation in environmental conditions. Even isolated enzymes cannot be used over a wide range of temperature, as proteins thermally denature at relatively low temperatures. The conditions that support life therefore dictate the reaction conditions in biochemical reactors, and a particular biochemical reaction will usually be constrained to relatively narrow ranges of temperature, shear rate, concentration of oxygen, and other solutes and pH. The optimal range of these conditions depends on the organism or enzyme chosen. Almost all biological processes are carried out in an aqueous solvent, and most are operated at temperatures slightly above ambient. The design of bioreactors is discussed in more detail in Section 15.9.

15.4.2 Catalyst

A catalyst increases the rate of a chemical reaction without itself becoming permanently changed by the reaction. By increasing the reaction rate, catalysts allow reactions to be run in smaller reactors, or in some cases allow a reaction to be operated at lower temperature. Most important of all, catalysts can be found that are more selective for a desired reaction, and hence the desired reaction can be promoted relative to other reactions and the process selectivity can be improved.

Catalytic reactors are discussed in more detail in Section 15.8. If a catalyst that is selective for the desired reaction can be found, it will almost always lead to a more economically attractive process than a noncatalytic route. Much of the research and development effort of the chemical industry therefore goes into searching for better catalysts.

The use of a catalyst usually introduces additional constraints into the selection of reactor operating conditions. Regardless of whether the catalyst is homogeneous (same phase as the reagents) or heterogeneous (different phase from the reagents—usually a solid), the reactor conditions must maintain catalyst activity for a reasonable length of time between catalyst regenerations. Catalysts are in general less stable and more prone to deactivation at high temperatures. Catalysts can also be sensitive to feed contaminants and may impose constraints on the concentration of certain components that could be present in the feed or might accumulate in recycle streams.

15.4.3 Temperature

Higher temperatures always increase the rate of reaction, diffusivities, and mass transfer rates. Higher temperatures increase the equilibrium constant of endothermic reactions and decrease the equilibrium constant of exothermic reactions (Fig. 15.8), but it should be noted that many exothermic reactions have very high equilibrium constants even at high temperature.

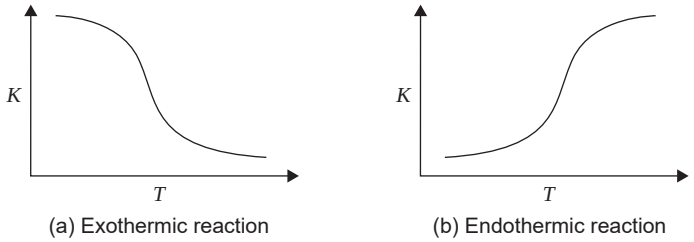


FIG. 15.8 Effect of temperature on equilibrium constant.

In general, increasing reaction temperature will lead to a less costly reactor design until one of the following constraints or trade-offs is encountered:

- Biological agents such as microorganisms, cells, and enzymes are killed or denatured at relatively low temperatures. Most biological processes are operated in the range 20 °C to 50 °C, and very few biological processes can be operated above 100 °C.
- Most organic compounds undergo thermal degradation reactions at high temperature. The presence of certain substituents, such as oxygen and nitrogen, can accelerate thermal degradation, and more complex molecular structures are typically more sensitive to pyrolysis. As temperature is raised, a point will be reached where thermal degradation will begin to have a detrimental effect on reactor selectivity. Some organic compounds can be sensitive to thermal decomposition at temperatures as low as 100 °C.
- At higher temperatures it can be harder to suppress side reactions such as polymerization or auto-oxidation. These reactions can pose a safety hazard, as well as reducing selectivity.
- The selectivity of oxidation reactions (and exothermic reactions in general) usually decreases as temperature is increased, as it becomes harder to maintain locally optimal concentrations of feed, oxidant, and product, and thus the tendency to oxidize the product increases. Selective oxidation reactions are therefore usually operated at as low a temperature as is practical and often use solvents or diluents to reduce the impact of the reaction exotherm.
- It is more difficult to maintain temperature control of exothermic reactions at high temperature, and there is a greater potential for the reaction to run away. Safety considerations in the design of reactors for exothermic processes are discussed in Section 15.13.
- At very high temperatures the cost of constructing a reactor becomes prohibitive. Maximum allowable stresses for steels start to decrease significantly with temperature above 300 °C. The pressure vessel design codes limit the maximum temperature at which alloys can be used; see Section 6.3.7. For reactions carried out under pressures greater than about 70 bar, an important threshold is reached at 482 °C (900 °F), as this is the maximum temperature limit for using the ASME Boiler and Pressure Vessel Code Section VIII Division 2 design rules. Any vessel operating with a wall temperature above this limit would need to be designed under the more conservative (hence higher cost) Division 1 rules. Higher temperatures can be accommodated by using *cold-wall* reactors, in which the reactor is lined with refractory material to reduce the temperature at the pressure-retaining wall, but this approach leads to larger reactors, and cold-wall reactors must be inspected regularly to ensure integrity of the lining.

15.4.4 Pressure

Several factors must be considered in selecting the reactor pressure. The primary consideration is usually to ensure the reactor contents are in the desired phase under the temperature conditions selected.

In some cases, the pressure is chosen so as to allow or prevent vaporization of a component. For example, it may be advantageous to allow a product to evaporate during the reaction so that it can be recovered from the vapor phase. Alternatively, in some cases a stoichiometric by-product can be allowed to evaporate, causing the equilibrium of the main reaction to be shifted. Feed, product, or solvent are sometimes allowed to evaporate as a means of removing heat from the reactor.

For gas-phase reactions, increasing the reactor pressure has the effect of increasing reactant activity, and hence increases the reaction rate. For reactions that are approaching equilibrium, the reactor yields change in accordance with Le Chatelier's principle. If the reaction leads to an increase in total number of moles, then a higher equilibrium conversion will be obtained at low pressure. Conversely, if the reaction leads to a reduction in total number of moles, then the equilibrium conversion will be higher at high pressure.

For gas–liquid reactions, increasing pressure will increase the solubility of the gas-phase components in the liquid, increasing the reaction rate. The effect of pressure on mass transfer rate is usually small. The savings in reactor cost resulting from higher gas solubility will, however, often be negligible compared with the increased

cost of compressing the gas. An additional important benefit of high-pressure operation is that less liquid will be lost by evaporation into any gas that is vented from the process. The savings in vent gas recovery equipment from operating at higher pressure are often greater than the savings in reactor cost.

15.4.5 Reaction phase

Reactions are usually not carried out in the solid phase unless the reagent is an insoluble solid such as coal, wood pulp, mineral ore, recycled polymer, etc. Fluids are easier to handle, compress, meter (flow control), heat and cool, and transport between process operations. Solid-phase reagents or products such as cells, polymer beads, and minerals are usually suspended in a gas or liquid for reaction.

The reaction temperature often dictates the reaction phase. In general, operation in the liquid phase gives the highest concentrations and most compact reactor, but at temperatures above the critical temperature, it is not possible to form a liquid phase. If all the reacting components cannot be maintained in the liquid phase at a reasonable pressure, a multiphase reactor will be needed, which will introduce mass transfer resistances and require a reactor with high vapor–liquid interfacial area; see Section 15.8. In some cases it will then make sense to decrease the pressure to the point where the reaction temperature is above the dew point and the reaction can be carried out in the vapor phase.

Some reaction systems are designed to operate with two liquid phases. Liquid–liquid reactors can have several advantages over single liquid-phase reactors and are discussed in more detail in Section 15.7.2.

15.4.6 Solvent

Many liquid-phase reactions are carried out with the reacting components dissolved in an inert solvent. A solvent can serve several purposes:

- Dilution of feed components to reduce the rates of side reactions and improve selectivity
- Increasing the solubility of gas-phase reactants
- Allowing components that would otherwise be solids to be dissolved in the reacting phase
- Increasing thermal mass and reducing the temperature change due to reaction
- Bringing components that would be mutually insoluble together so that they can react

A good solvent should be inert to the main reaction and to reactions with by-products and feed contaminants. A good solvent should also have low cost, should be easily separated from the reaction products, and should not introduce serious safety or environmental concerns. Properties of some of the solvents that are most widely used in the process industries are given in Table 15.4.

TABLE 15.4 Commonly used process solvents

Solvent	Advantages	Disadvantages
Water	• Low cost, readily available • Easy and inexpensive to dispose of waste • Nontoxic, not flammable • Natural environment for most biological agents • Strong polar solvent (dielectric constant = 80.1) with ability to hydrogen bond, hence high solubility for many organic and inorganic compounds • High density allows easy separation from insoluble organic liquids, enabling liquid–liquid separations • High specific heat capacity gives high thermal mass and moderates temperature change due to heat of reaction, making temperature control easier • Remains liquid over a broad range of temperature at moderate pressures	• Presence of ions can make water corrosive • Low solubility for many nonpolar organic compounds • Presence of salts or ions can cause unwanted formation of second liquid phase • Heterogeneous catalysis can be more difficult in aqueous phase (due to leaching, galvanic effects, etc.) • Forms azeotropes with many compounds, making downstream separations more difficult • Reactive with many compounds • High latent heat can make recovery by distillation energy intensive • Contaminated water must be carefully handled to prevent mixing with groundwater

TABLE 15.4 Commonly used process solvents—cont'd

Solvent	Advantages	Disadvantages
Light alcohols (methanol, ethanol, n-propanol, isopropanol)	• Low-cost commodity chemicals • Moderate polar solvents (dielectric constants MeOH = 33, EtOH = 25, n-PrOH = 20, i-PrOH = 18) with ability to hydrogen bond • Liquid over broad range of temperature at moderate pressures, but easily recovered by fractionation as long as azeotropes are not present	• Toxic • Flammable • Tendency to form azeotropes with water and oxygenated compounds (except methanol), requiring more complex distillation for solvent recovery • Easily oxidized to aldehydes and acids (except isopropanol)
Acetic acid	• High-dipole moment makes acetic acid a good polar solvent, despite low dielectric constant (6.2). • Able to hydrogen bond • Resistant to oxidation, so widely used as solvent in oxidation reactions • Can be recovered by fractionation at moderate temperatures	• Toxic • Corrosive in presence of water • Flammable • Tendency to form azeotropes with other oxygenated compounds
Acetone	• Good polar aprotic solvent with high solubility for many organic compounds, including polymers • Miscible with water • Low chronic and acute toxicity in normal use	• Flammable with low flash point (−20 °C) and broad range of flammability in air, so easily ignited
Acetonitrile	• Medium polarity solvent (dielectric constant 37.5) with ability to dissolve many electrolytes as well as organic compounds • Low viscosity; hence widely used in chromatography	• Flammable • Moderate toxicity because acetonitrile is metabolized to hydrogen cyanide
Diethyl ether	• Good nonpolar solvent with high solubility for many organic compounds • Low solubility in water allows liquid−liquid extraction of products • Low toxicity in normal use	• Low autoignition temperature (160 °C) and flash point (−45 °C) make ether highly flammable • Prone to formation of explosive peroxides
Halogenated solvents (e.g., chloroform, dichloromethane, fluorinated solvents)	• Variation of the type and extent of halogenation allows a wide range of compounds to be developed with the ability to tailor polarity and volatility to specific needs • Reactivity with other compounds is usually low • Generally can be designed to be nonflammable and nontoxic • High density, allowing easier separation from insoluble liquids	• Some halogenated solvents (e.g., chloroform) are carcinogenic • Disposal costs can be high due to concerns about dioxin formation if incinerated, global warming potential
Benzene	• Good nonpolar solvent with low reactivity and low solubility in water, but highly carcinogenic and so usually substituted with toluene, cyclohexane, or other solvents whenever possible	• Flammable • Toxic, carcinogenic, and highly regulated
Toluene	• Low polarity • Low miscibility with water • More reactive than benzene, but much less toxic, so preferred over benzene as aromatic solvent	• Toxic • Flammable • Possible teratogen
Cyclohexane	• Low polarity • Low miscibility with water • Low reactivity with many compounds	• Extremely flammable (flash point −20 °C, autoignition temperature 245 °C) • Toxic (causes skin and lung irritation)
Paraffins (pentane, hexane, decane, etc.)	• Low polarity, only dissolve nonpolar compounds • Low miscibility with water • Inexpensive • Low reactivity with many compounds • Low acute toxicity	• Flammable • Volatility varies with carbon number, but light paraffins are easily vaporized and ignited

Note: Consult individual MSDS forms for additional safety information, including chemical incompatibility.

In some cases, a solvent can be found that will allow reaction and separation to be carried out simultaneously. For example, if the reaction feeds are soluble in the solvent but the product is not, product can be precipitated and removed continuously, shifting the equilibrium of the reaction to full conversion.

When selecting a solvent, care must be taken to ensure that the solvent will be compatible with all the components present in the reacting mixture. Some common solvents can be highly reactive with components such as oxidizing agents.

15.4.7 Concentrations

The concentration of components in the liquid phase can be increased up to the limit of solubility in the solvent, although operation at the limit of solubility is usually avoided to prevent problems due to precipitation or formation of a second liquid phase. The concentration of components in the gas phase (partial pressure) can be increased by increasing system pressure.

Feeds

Higher concentrations of feed compounds usually lead to a higher rate of reaction and a smaller reactor. In some situations, such as highly exothermic reactions, high concentrations should be avoided, in which case either a large excess of one feed is used or an inert material is added, as described next.

Feed components do not need to be supplied in stoichiometric ratio, and in fact very few processes use a stoichiometric ratio of feeds. Using a higher concentration of one feed can improve the selectivity of a reaction or the conversion of another compound. For example, the alkylation of benzene with propylene to form cumene is usually carried out with excess benzene. This increases the reaction selectivity by reducing the formation of diisopropyl- and triisopropyl-benzene, while also allowing full conversion of propylene and obviating propylene recovery for recycle.

By-products and contaminants

The concentrations of all possible feed contaminants and by-products are important variables that must be understood by the reactor designer and the research team. The effect of these components on catalysts and reaction rates can play a critical role in determining reactor performance and overall selectivities. It is very important to ensure that reactor performance has been tested under conditions that are representative of the expected levels of these components, particularly when recycle streams are present.

It may be advantageous to allow some by-product species to be recycled to the reactor. If the by-products are formed through reversible reactions that are not part of the desired reaction stoichiometry, they can be recycled to extinction, leading to greater overall selectivity to the desired product. Allowing some buildup of by-products in recycles can also sometimes suppress the rate of by-product formation. Allowing some buildup of by-products in a feed recycle can significantly reduce the cost of downstream separation processes.

Feed contaminants are generally more problematic than by-products, particularly for biological and catalytic processes. The feeds to fermentation reactors must be sterilized to prevent contamination by bacteria, viruses, fungal spores, etc.; see Section 15.9.3. Catalysts can be sensitive to poisons such as metals, compounds containing sulfur, oxygen or nitrogen, carbon monoxide (which adsorbs strongly on noble metals), and even water, which can strongly adsorb on solid acid catalysts. Compounds that have a tendency to form carbonaceous deposits on a catalyst (coke precursors) will accelerate the rate of catalyst deactivation by coking if they are allowed to accumulate in recycle streams.

If the effect of a feed contaminant is known to be particularly severe, the design should be modified to remove the contaminant upstream of the reactor. This may be as simple as adding a guard bed of a suitable adsorbent, as described in Section 16.2.1, or may require a more complex treatment process.

Inerts

The addition of inert compounds to a reacting mixture will usually increase the reactor cost, as well as adding downstream separation costs; however, there are some situations where it may still be worthwhile:

- The addition of an inert compound to a gas-phase reaction reduces the partial pressure of the reagents. This can increase the equilibrium conversion in reactions that lead to an increase in number of moles.
- Diluents can reduce the rate of reaction of a feed compound with itself, or with products, and thereby increase selectivity.

- Addition of an inert diluent can allow operation outside the flammability envelope. Oxygenation reactions are often carried out using depleted air (enriched in nitrogen) to reduce the likelihood of forming a flammable mixture.
- The presence of a diluent increases the heat capacity flow rate ($m.C_p$) of the mixture, and hence reduces the change in temperature caused by the heat of reaction. Moderation of the change in temperature has safety benefits for exothermic reactions and reduces the number of reheats required in endothermic reactions. It can also help prevent the formation of hot or cold spots in the reactor.
- Inert compounds are sometimes added to solutions to buffer the solution and allow more stable control of pH or ionic strength.

One of the best-known examples of use of a diluent is the use of steam in ethylene cracking furnaces, where the steam reduces the feed partial pressure, suppresses side reactions, and also suppresses coking.

15.5 Mixing

In addition to playing a critical role in reactor performance, mixing processes are important in many other processing stages, from the preparation of reagents through to the final blending of products. The equipment used depends on the nature of the materials and the degree of mixing required.

In many processes, some or all of the reactor feeds are premixed before being pumped to reactor pressure and heated to reaction temperature. Premixing is commonly used when solid feeds must be dissolved or fed as a slurry, and liquid and solids mixing operations are often carried out as batch processes.

This section addresses the mixing of fluids and mixing of solids into fluids. The blending of mixtures of dry solids is addressed in Section 18.4.11. An overview of scale-up rules for mixing is given by Post (2010).

15.5.1 Gas mixing

Specialized equipment is rarely needed for mixing gases, which because of their low viscosities mix easily. The mixing given by turbulent flow in a length of pipe is usually sufficient for most purposes. Turbulence promoters, such as orifices, vanes, or baffles, can be used to increase the rate of mixing. The piping arrangements used for inline mixing are discussed in the section on liquid mixing.

15.5.2 Liquid mixing

The following factors must be taken into account when choosing equipment for mixing liquids:

1. Batch or continuous operation
2. Nature of the process: miscible liquids, preparation of solutions, or dispersion of immiscible liquids
3. Degree of mixing required
4. Physical properties of the liquids, particularly the viscosity
5. Whether the mixing is associated with other operations such as reaction or heat transfer

Inline mixers can be used for the continuous mixing of low-viscosity fluids. For other mixing operations, stirred vessels or proprietary mixing equipment will be required.

Inline mixing

Static devices that promote turbulent mixing in pipelines provide an inexpensive way of continuously mixing fluids. Some typical designs are shown in Fig. 15.9. A simple mixing tee (see Fig. 15.9a), followed by a length of pipe equal to 10 to 20 pipe diameters, is suitable for mixing low-viscosity fluids ($\leq$50 mNs/m^2), providing the flow is turbulent and the densities and flow rates of the fluids are similar.

With injection mixers (see Figs. 15.9b and c), in which the one fluid is introduced into the flowing stream of the other through a concentric pipe or an annular array of jets, mixing will take place by entrainment and turbulent diffusion. Such devices should be used where one flow is much lower than the other and will give a satisfactory blend in about 80 pipe diameters. The inclusion of baffles or other flow restrictions will reduce the mixing length required.

The static inline mixer shown in Fig. 15.10 is effective in both laminar and turbulent flow and can be used to mix viscous mixtures. The division and rotation of the fluid at each element cause rapid radial mixing; see Rosennzweig

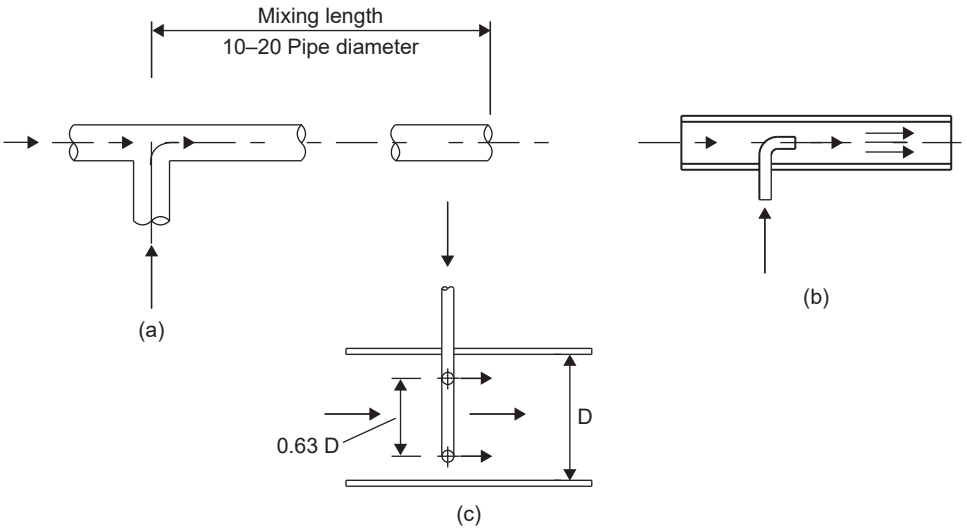


FIG. 15.9 Inline mixers. (a) Tee. (b) Injection. (c) Annular.



FIG. 15.10 Static mixer. *Courtesy Kenics Corporation.*

(1977) and Baker (1991). There is a great variety of different proprietary designs for static mixers, and they are easily found by searching on the Internet. The dispersion and mixing of liquids in pipes is discussed by Zughi et al. (2003) and Lee and Brodkey (1964).

Centrifugal pumps are effective inline mixers for blending and dispersing liquids. Various proprietary motor-driven inline mixers are also used for special applications; see Green and Southard (2018).

Stirred tanks

Mixing vessels fitted with some form of agitator are the most commonly used type of equipment for blending viscous liquids and preparing solutions of dissolved solids.

The stirred tank reactor can also be considered to be the basic chemical reactor, modeling on a large scale the conventional laboratory flask. Tank sizes range from a few liters to several thousand liters. They are used for homogeneous and heterogeneous liquid–liquid and liquid–gas reactions and for reactions that involve finely suspended solids, which can be held in suspension by the agitation. As the degree of agitation is under the designer's control, stirred tank reactors are particularly suitable for reactions where good mass transfer or heat transfer is required.

Most stirred tank reactors are not designed to operate completely filled with liquid. A vapor space is left at the top of the vessel to make pressure control easier. Stirred tanks should not be designed to operate more than 90% full, and 60% to 70% full is most typical. Lower liquid levels are used in reactors that have gas feeds (to allow for droplet disengagement) or are prone to foaming.

Liquid mixing in stirred tanks is covered in several textbooks: Uhl and Gray (1967), Harnby et al. (1997), Tatterson (1991, 1993), McCabe et al. (2004), Chhabra and Shankar (2017), and Paul et al. (2003).

A typical arrangement of the agitator and baffles in a stirred tank, and the flow pattern generated, is shown in Fig. 15.11. Mixing occurs through the bulk flow of the liquid and, on a microscopic scale, by the motion of the turbulent eddies created by the agitator. Bulk flow is the predominant mixing mechanism required for the blending of miscible liquids and for solids suspension. Turbulent mixing is important in operations involving mass and heat transfer, which can be considered as shear-controlled processes.

The most suitable agitator for a particular application will depend on the type of mixing required, the capacity of the vessel, and the fluid properties, mainly the viscosity.

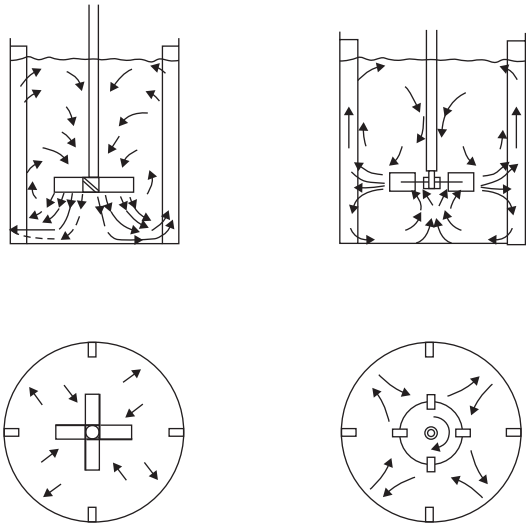


FIG. 15.11 Agitator arrangements and flow patterns.

The three basic types of impeller that are used at high Reynolds numbers (low viscosity) are shown in Fig. 15.12. They can be classified according to the predominant direction of flow leaving the impeller. The flat-bladed (Rushton) turbines are essentially radial-flow devices, suitable for processes controlled by turbulent mixing (shear-controlled processes). The propeller and pitched-bladed turbines are essentially axial-flow devices, suitable for bulk fluid mixing.

Paddle, anchor, and helical ribbon agitators (Fig. 15.13) and other special shapes are used for more viscous fluids.

The selection chart given in Fig. 15.14, which has been adapted from a similar chart given by Penny (1970), can be used to make a preliminary selection of the agitator type, based on the liquid viscosity and tank volume. Impeller selection is also discussed in the articles by Fasano (2015) and Grenville et al. (2017). Specially designed impellers are used in situations when high shear is needed, such as when dispersing fine powders into a liquid. See Dickey (2015) for examples.

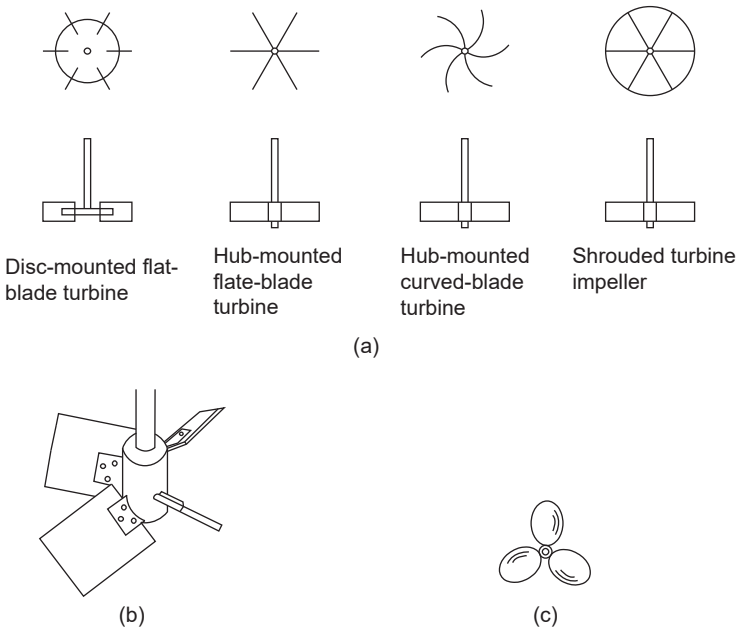


FIG. 15.12 Basic impeller types. (a) Turbine impeller. (b) Pitched bladed turbine. (c) Marine propeller.

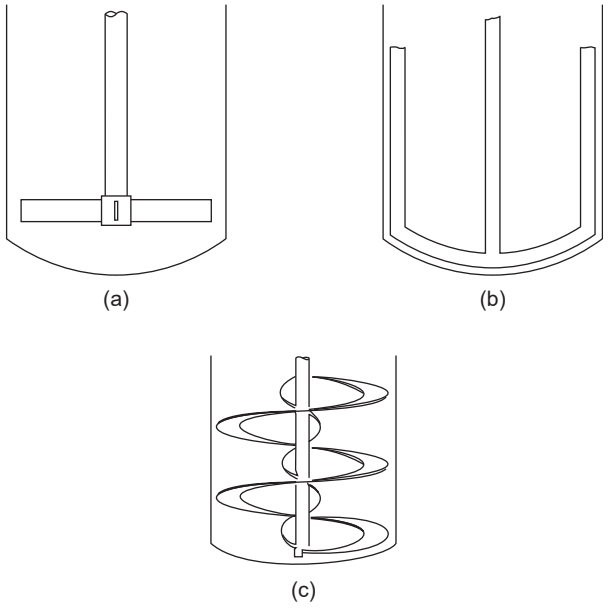


FIG. 15.13 Low-speed agitators. (a) Paddle. (b) Anchor. (c) Helical ribbon.

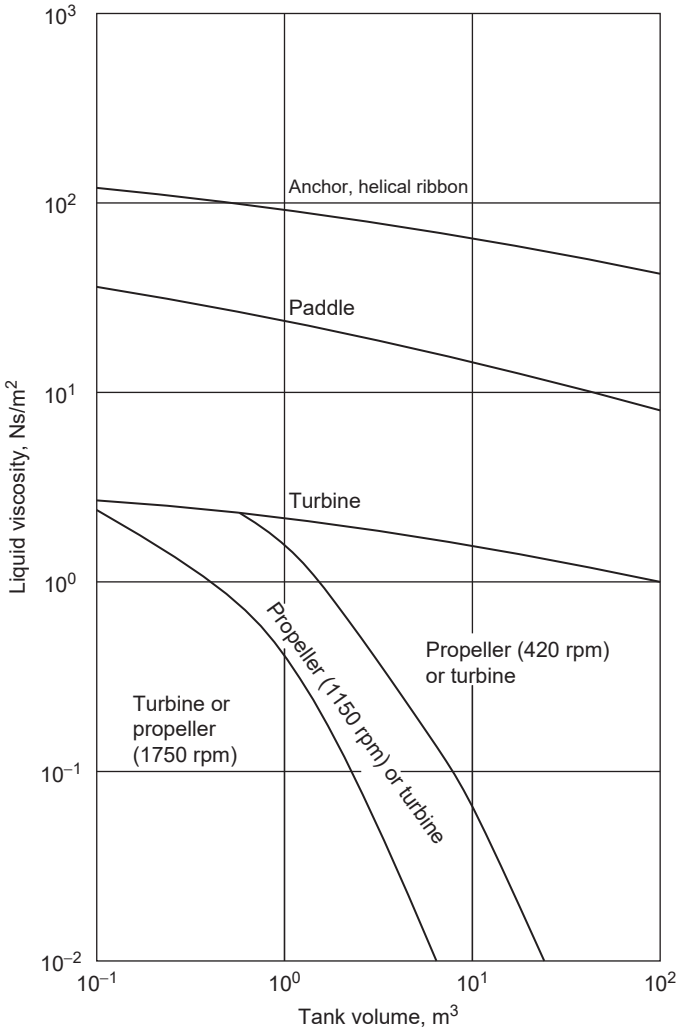


FIG. 15.14 Agitator selection guide.

For turbine agitators, impeller—to—tank diameter ratios of up to about 0.6 are used, with the depth of liquid equal to the tank diameter. Baffles are normally used to improve the mixing and reduce problems from vortex formation. Anchor agitators are used with close clearance between the blades and vessel wall, with anchor—to—tank diameter ratios of 0.95 or higher. The selection of agitators for dispersing gases in liquids is discussed by Hicks (1976).

Agitator power consumption

The power requirements for agitation will depend on the degree of agitation required and will range from about 0.2 kW/m^3 for moderate mixing to 2 kW/m^3 for intense mixing.

The shaft power required to drive an agitator can be estimated using the following generalized dimensionless equation, the derivation of which is given in Chhabra and Shankar (2017).

$$\mathrm{N_p} = K\mathrm{Re}^b\mathrm{Fr}^c \tag{15.16}$$

where:

$\mathrm{N_p}$ = power number = $\frac{P_a}{d_a^5 N^3 \rho}$
Re = Reynolds number = $\frac{d_a^2 N \rho}{\mu}$
Fr = Froude number = $\frac{d_a N^2}{g}$
P_a = shaft power, W
K = a constant, dependent on the agitator type, size, and the agitator tank geometry
ρ = fluid density, kg/m^3
μ = fluid viscosity, Ns/m^2
N = agitator speed, s^{-1} (revolutions per second, rps)
d_a = agitator diameter, m
g = gravitational acceleration, 9.81 m/s^2

Values for the constant K and the indices b and c for various types of agitator, tank agitator geometries, and dimensions can be found in the literature; see Rushton et al. (1950). A useful review of the published correlations for agitator power consumption and heat transfer in agitated vessels is given by Wilkinson and Edwards (1972); they include correlations for non-Newtonian fluids. Typical power curves for propeller and turbine agitators are given in Figs. 15.15 and 15.16. In the laminar flow region, the index "b" = 1, and at high Reynolds number the power number is independent of the Froude number: index "c" = 0.

An estimate of the power requirements for various applications can be obtained from Table 15.5.

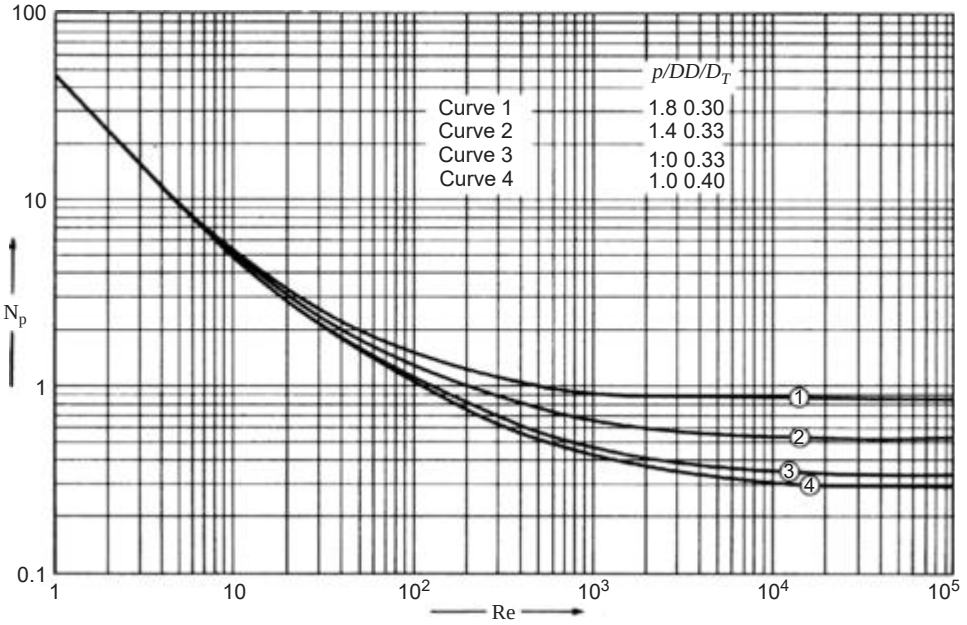


FIG. 15.15 Power correlation for single three-bladed propellers baffled. p = blade pitch, D = impeller diameter, DT = tank diameter. *From Uhl & Gray, 1967, with permission.*

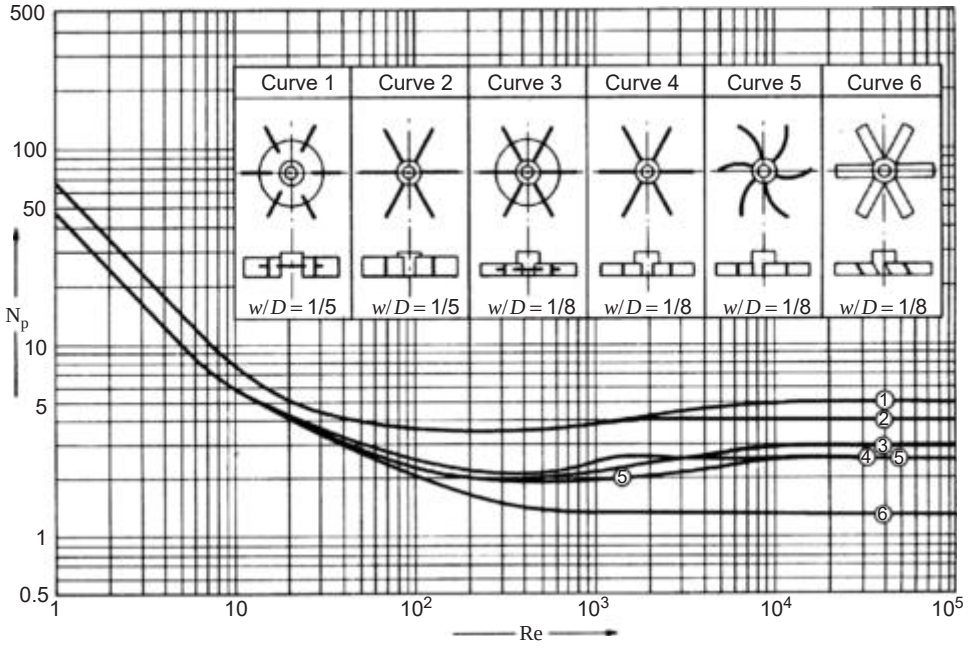


FIG. 15.16 Power correlations for baffled turbine impellers for tank with four baffles. w = impeller width, D = impeller diameter. *From Uhl & Gray, 1967, with permission.*

TABLE 15.5 Power requirements: Baffled agitated tanks

Agitation	Applications	Power, kW/m^3
Mild	Blending, mixing	0.04–0.10
	Homogeneous reactions	0.01–0.03
Medium	Heat transfer	0.03–1.0
	Liquid–liquid mixing	1.0–1.5
Severe	Slurry suspension	1.5–2.0
	Gas absorption	1.5–2.0
	Emulsions	1.5–2.0
Violent	Fine slurry suspension	>2.0

Side-entering agitators

Side-entering agitators are used for blending low-viscosity liquids in large tanks, where it is impractical to use conventional agitators supported from the top of the tank; see Oldshue et al. (1956).

Where they are used with flammable liquids, particular care must be taken in the design and maintenance of the shaft seals, as any leakage may cause a fire.

For blending flammable liquids, the use of liquid jets should be considered as an "intrinsically" safer option; see Fossett and Prosser (1949).

15.5.3 Gas–liquid mixing

Gases can be mixed into liquids using either inline mixing, stirred vessels, or the vapor–liquid contacting devices described in Chapter 17.

When a small amount of gas is fed or the gas dissolves completely, inline mixing can be used. The most common arrangement is an injection mixer (see Fig. 15.9b) followed by a static mixer. In some cases, a long injection tube with multiple holes drilled in it is used. This is known as a *sparger* (Fig. 15.17).

If a gas is injected into a stirred tank, the location of the gas injection must be chosen based on the mixing pattern obtained with the impeller that has been selected. The gas injection device is usually an annular ring with multiple small openings, and the openings are oriented to promote the desired circulation of gas bubbles. Methods such as computational fluid dynamics (CFD) are used to analyze the gas bubble flow pattern and ensure that the gas hold-up and interfacial area are adequate; see Section 15.11.3. The rate of mass transfer from gas to liquid can be predicted using Equations 15.13 to 15.15. It should always be assumed that any excess vapor leaving a stirred tank will be saturated with all the components of the liquid, and it is reasonable to assume at least 1 to 2 volume percent entrainment of liquid in the vapor if the rate of agitation is high.

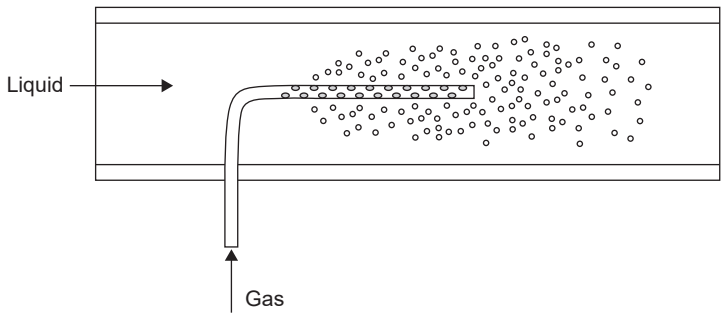


FIG. 15.17 Gas sparger.

The extent of agitation caused by injecting a gas into a liquid can be seen from Table 15.6, which is based on information from Green and Southard (2018).

A small flow of liquid can be dispersed into a gas stream using a spray nozzle (Fig. 15.18). Many different proprietary spray nozzles are available, and the nozzle is usually selected in consultation with a vendor.

When large flow rates of vapor and liquid are to be contacted to carry out reaction, mass transfer, or direct heat transfer, plate or packed columns are usually used; these are discussed in detail in Chapter 17.

TABLE 15.6 Air rate ($ft^3/ft^2.min$) required to cause agitation of water at 1 atm

Degree of agitation	Liquid depth 9 ft	Liquid depth 3 ft
Moderate	0.65	1.3
Complete	1.3	2.6
Violent	3.1	6.2

From Green and Southard (2018).

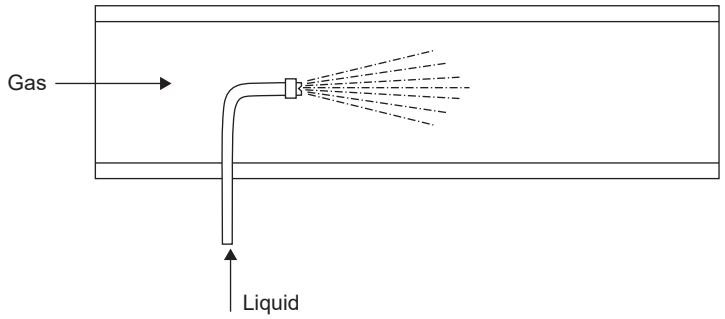


FIG. 15.18 Liquid injection into gas.

15.5.4 Solid–liquid mixing

Solids are mixed into liquids to dissolve solid feeds and to form slurries for transport and reaction of insoluble solids. Solids are usually added to a liquid in a stirred tank, although liquids are sometimes introduced into screw conveyors, which then act as mixing troughs. The design of stirred tanks is covered in Section 15.5.2.

Liquids and solids are usually mixed at atmospheric pressure to make handling and flow of the solid easier. The resulting mixture or slurry can then be pumped to the process pressure.

Mixing of liquids and solids is often carried out as a batch operation to allow more accurate control of dissolved solid concentration. A modest inventory of solution or slurry can then be used to maintain a constant feed to continuous downstream operations. If an inventory of slurry is maintained, it must be continuously agitated to prevent settling.

The formation of slurry feeds for hydraulic conveying is discussed in Section 18.3.5. Many of the same considerations apply when feeding a solid to a liquid-phase reactor.

15.6 Heating and cooling of reacting systems

Heat addition and removal are important for maintaining temperature control of exothermic and endothermic reactions. For endothermic reactions, the rate of heat input can sometimes be the rate-limiting step.

15.6.1 Heating and cooling reactors: Basic principles

Adding heating or cooling to a reactor design always increases the reactor cost. The designer should first consider the following:

1. Can the reaction be carried out adiabatically? If the heat of reaction is small, a small change in temperature across the reactor may be acceptable and heating or cooling can be avoided. If a diluent is added to the system, the thermal mass of the reagents will increase and the temperature change across the reactor will be reduced, so adding a diluent can enable adiabatic operation.
2. Can the feeds provide the required heating or cooling? Staged addition of hot feed to a reactor can provide additional heat to an endothermic reaction. Similarly, staged addition of cold feed can provide quench to an exothermic reaction. A commercial example of this is the use of hydrogen quenches to control the temperature increase during hydrocracking reactions (Fig. 15.19). In a stirred tank or other reactor that approximates well-mixed reactor behavior, the heat of reaction can sometimes be balanced by a sensible heat change between a hot or cold feed temperature and the reactor temperature.
3. Would it be more cost-effective to carry out the heat exchange outside the reactor? If the required heat transfer surface is large, it may be difficult to fit into a simple reactor design, in which case the designer should consider using an external heat exchange system. Examples are given in the following sections.
4. Would it be more effective to carry out the reaction inside a heat transfer device? If the required residence time is small, or if the volume of catalyst is small, the reaction can sometimes be carried out inside the tubes of a heat exchanger or fired heater. The use of heat-exchange devices as reactors is discussed in Section 15.6.4.
5. Does the proposed design allow the process to be started up and shut down smoothly? The heating or cooling system must be flexible to respond to nonsteady operating conditions of the plant, as well as steady-state operation.
6. Are there safety concerns with heating or cooling the reactor? For exothermic reactions, the designer should consider what would happen if there was a failure of the cooling system. How quickly can the control system respond and shut the reaction down before the exothermic reaction runs away? Exothermic reactors should not require a heater, and feedback between feed heaters, feed-effluent heat exchangers and the reactor must be considered. Are there concerns about the heat transfer medium leaking into the reactor or reactor contents leaking into the heat transfer medium?

The heating or cooling duty of the reactor is usually most easily estimated using commercial process simulation software. The designer must take care to ensure that the enthalpy of reaction and the heat capacities used by the simulator are sufficiently accurate for design purposes; see Section 15.3.1.

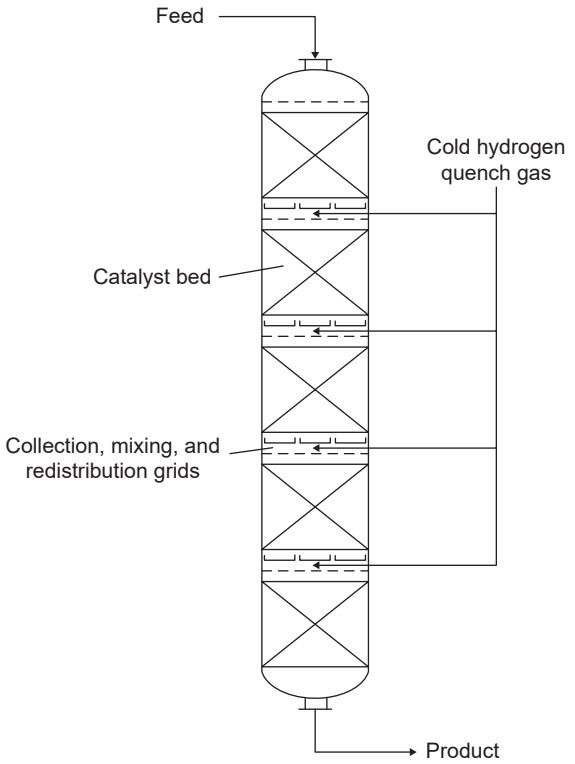


FIG. 15.19 Use of hydrogen quench in hydrocracking reactor.

Novice designers often make the mistake of forgetting to pre-heat (or pre-cool) the reactor feeds, leading to unreasonably large reactor heating or cooling duties. The reactor feed should be at the desired reaction temperature unless hot or cold feed is being used as a temperature control strategy.

15.6.2 Heating and cooling stirred tank reactors

A stirred tank reactor can be operated in batch or continuous mode. In either case, the objective in heating or cooling the contents is to achieve a uniform temperature throughout the vessel and eliminate hot or cold spots that could cause fouling, nonselective reaction, or lead to hazards such as reaction runaway. The heating or cooling should be accomplished without disrupting the mixing in the vessel and creating undermixed zones or dead spots.

Indirect heat transfer

Heat transfer to stirred vessels is described in detail in Section 19.18, and correlations for heat transfer coefficients are given in Section 19.18.3.

Fig. 15.20 shows the most common approaches to providing heating or cooling to stirred vessels. Low heating duties can be accommodated with a jacketed vessel (see Fig. 15.20a). The mechanical and thermal design of jacketed vessels is discussed in Section 19.18.1. Different utility flow patterns can be accommodated in a jacketed vessel. For

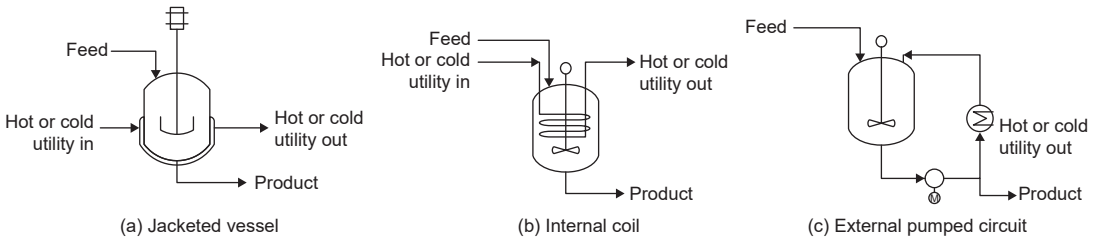


FIG. 15.20 Heating or cooling stirred-tank reactors.

example, when steam is used for heating a reactor, the steam usually flows in at the top of the jacket and condensate is drained near the bottom, whereas cooling water is usually fed from the bottom up.

If the area of a jacket is insufficient, an internal coil can be used (see Fig. 15.20b). Heat transfer to internal coils and coil pressure drop are covered in Section 19.18.2. Although coils can provide much more area, the volume of the reactor must be increased to accommodate the coil, and coils can be difficult to clean and sterilize.

For high rates of heat addition or removal, an external pumped circuit should be considered, as shown in Fig. 15.20(c). The use of an external heat exchanger removes any volume limit on accommodating the heat transfer surface and allows the heat exchange to be optimized independently of reactor design considerations. The residence time of the fluid in the pump, piping, and heat exchanger should be subtracted from the required residence time of the reactor. If a shell and tube heat exchanger is used, the reacting fluid will usually (but not always) be placed on the tube side to minimize the likelihood of forming dead spots or undermixed zones. Plate heat exchangers are often used in reactor pump-around circuits because of their low inventory of fluid, short residence time, and ease of cleaning.

In any reactor that uses indirect heat transfer, the designer must check carefully to ensure that local hot spots or cold spots on the heat transfer surface will not lead to fouling, excessive corrosion, or poor reaction selectivity. A calculation of the hottest and coldest metal surface temperatures should be made. These will normally be in regions close to where the utility enters and exits. The calculation can be based on a sophisticated model of reactor hydrodynamics, as described in Section 15.11.3, or can be as simple as an estimate based on internal and external heat transfer coefficients with suitably conservative assumptions. If there is a concern that either the hottest or coldest surface temperature could have a serious impact on reactor performance, the designer should reconsider the choice of hot or cold utility to attempt to reduce the temperature difference between the utility and reactor contents. This will generally lead to an increase in required area and may cause the selection of a different reactor design.

Direct heat transfer: Heating using live steam

If the reacting mixture is compatible with addition of water and the temperature and pressure are suitable, direct heat transfer to a vessel can be accomplished by injecting live steam into a reactor (Fig. 15.21). Steam is usually injected through a distribution ring or sparger, but if the vessel is well agitated, a simple dip tube may suffice.

The use of live steam eliminates the need for heat transfer surface and saves capital cost in the reactor. The trade-off is that the steam is lost to the process fluid and condensate cannot be recovered, so the cost of live steam must include the cost of replacing the boiler feed water. Process wastewater costs are also increased.

When live steam is used, it is unlikely that all the steam will condense, so provision must be made for a net vapor flow from the reactor. Any vapor leaving the reactor will be saturated with all the components of the reacting mixture, so the off-gas will normally be cooled and condensed to recover material that was vaporized. The cost impact of adding a vapor recovery system must also be considered when evaluating use of live steam if such a system was not already in place.

Direct heat transfer: Evaporative cooling

If the process feed, solvent, or product can be made to evaporate at the reaction temperature, evaporative cooling can be used to cool the reactor.

In an evaporative cooling system, the vapor from the reactor is usually cooled externally and condensed to recover process fluids. In some cases, two stages of cooling are used, with an air or water cooler followed by a refrigerated chiller. The condensed fluid is usually refluxed to the reactor to provide additional cooling (Fig. 15.22).

If the overhead system has adequate capacity, evaporative cooling can provide highly sensitive temperature control. A small decrease in pressure will quickly cause more evaporation and remove heat from the reactor, so the reactor temperature control can be cascaded onto the pressure control.

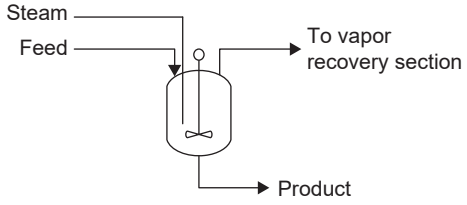


FIG. 15.21 Live steam injection.

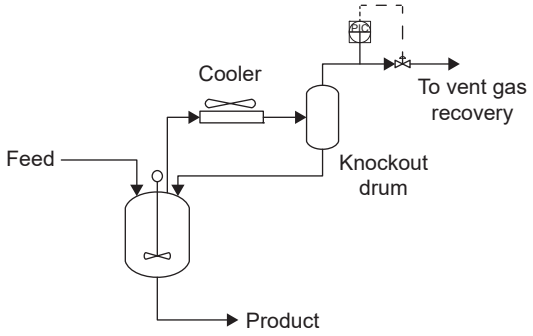


FIG. 15.22 Evaporative cooling.

15.6.3 Heating and cooling catalytic reactors

Slurry reactors

If a solid catalyst is mixed into a reacting liquid to form a slurry, heat transfer can be accomplished using the methods described in Section 15.6.2. Because slurries can cause erosion, the use of internal coils is not preferred. If an external pumped circuit is used, the pump design must be suitable for slurry service, and the fluid should be placed on the tube side of the exchanger to prevent filtering out of catalyst particles in dead spots. Plate heat exchangers can be used for slurries, but the designer should consult with a plate exchanger vendor to ensure that the gap spacing is adequate to prevent plugging.

Fixed-bed reactors

It is usually difficult to heat or cool a fixed-bed reactor by indirect heat transfer, as it is hard to maintain a uniform temperature profile across a radial section of the bed. Radial variation in temperature can cause faster deactivation of catalyst in the hotter zones and shorten the time between plant shutdowns for catalyst change-out.

The most common approach for heating or cooling a fixed-bed reactor is to divide the reactor into a series of smaller adiabatic beds and use interstage heating or cooling, as shown in Fig. 15.23. Each bed is sized to have an acceptable adiabatic change in temperature. In the case of an endothermic reaction, the inlet temperature must not be so hot that selectivity is compromised, whereas the outlet temperature must be hot enough to maintain

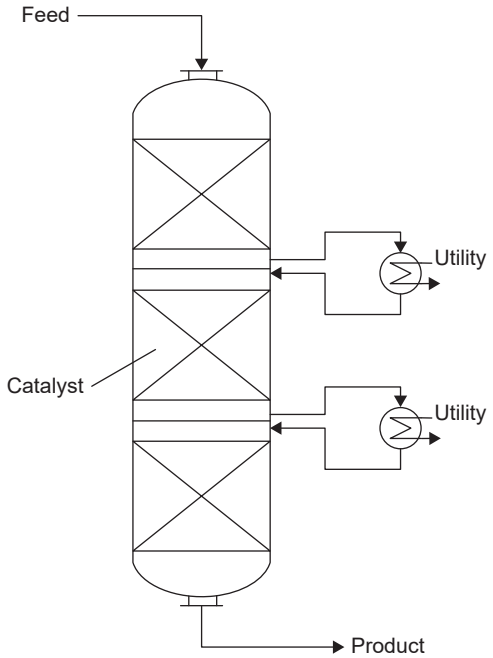


FIG. 15.23 Fixed-bed reactor with interstage heating or cooling.

reasonable catalyst activity. For an exothermic reaction, the situation is reversed, and care must be taken to ensure that the reaction will not run away at the outlet temperature. The bed sizes are not necessarily equal, as the reaction rate may vary from bed to bed.

In scaling up nonisothermal packed-bed reactors, the designer must ensure that the temperature change across each bed remains about the same as the capacity is increased. Because the temperature across any given bed is not uniform, both the bed inlet temperature and the average bed temperature should be kept the same during scale-up.

Occasionally, it will be possible to pack the catalyst into tubes of a heat exchanger or fired heater. The use of heat-exchange devices as reactors is discussed in Section 15.6.4.

Fluidized-bed reactors

Fluidized beds have high heat transfer coefficients; see Zenz and Othmer (1960). Indirect heat transfer to fluidized-bed reactors using coils or stab-in heat exchange bundles is therefore often effective.

The heat capacity of the solids in a fluidized bed allows the solid particles themselves to be used as a heat transfer medium. In processes such as fluidized catalytic cracking (FCC), the catalyst is heated to a temperature above the reaction temperature in a regeneration reactor. Hot catalyst is then circulated back to the reactor, where it provides the heat of reaction and heat needed to vaporize the feed. Deactivated catalyst is returned to the regeneration reactor. This process is discussed in more detail in Section 15.8.4 and illustrated in Fig. 15.42.

15.6.4 Heat-exchange devices as reactors

When it is necessary to operate a reactor isothermally and there is a large heat of reaction, the heat transfer requirements dominate the design, and the reactor must be designed as a heat transfer device. Some common situations where this occurs include:

- High-temperature endothermic reactions that quickly quench without continuous heat input.
- Low-temperature exothermic reactions that must be kept at constant temperature to maintain selectivity or for safety reasons. Many selective oxidation reactions fall into this category.

Reactions can be carried out inside any heat transfer device, but the most commonly used arrangements are shell and tube heat exchangers or fired heaters. Plate heat exchanger reactors have been the subject of much research, but are not yet in widespread commercial use.

Homogeneous reaction

If the reaction mixture is a single phase and there is no need for a catalyst, then the mechanical design and layout of a heat exchanger reactor is the same as a conventional heat transfer device. The thermal design of a heat exchanger reactor, however, is much more complex than a conventional heat exchanger.

The heat exchanger design equations that are normally used for heat transfer will not apply to the design of a heat exchanger reactor due to the nonlinear behavior of the reaction rate with temperature and hence the variation in heat release (or uptake) along the exchanger tubes. For example, in the case of an exothermic reaction, the rate of reaction might be expected to be highest at the inlet, where the concentrations of feeds are highest, but as the reaction proceeds and temperature increases, the rate of reaction will increase, so the hot spot in the tube may actually be at some distance in from the inlet, as illustrated schematically in Fig. 15.24. The location of the hot spot can be further complicated by the flow pattern on the shell side of the heat exchanger; hence determination of the effective temperature difference for the exchanger is not trivial. Many shell and tube heat exchanger reactors are operated using a constant temperature utility such as boiling water or a boiling refrigerant as coolant to simplify the thermal design and ensure good control of utility-side temperature.

It is usually not wise to make a conservative assumption of the temperature difference and proceed with a standard heat exchanger design. A design with excessive area will not achieve the desired reaction temperature and, if placed in operation, may require changes in utility temperature that could compromise process safety margins. Although such an approach can be useful as a means of generating an approximate capital cost for the reactor in the early stages of design, great care must be taken to ensure that the design is revised before detailed design begins.

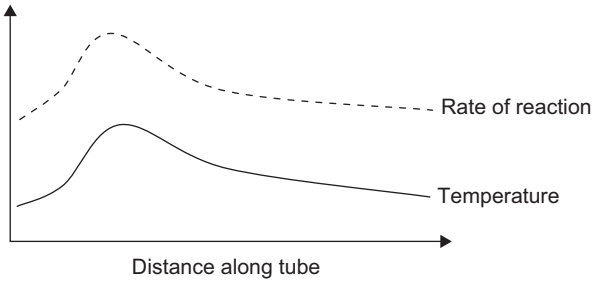


FIG. 15.24 Schematic profiles of temperature and reaction rate for an exothermic reaction in a heat exchange tube.

The approach that is typically followed in industrial practice is to construct a detailed model of the reaction kinetics and hydraulics, as described in Section 15.11.3. The model can then be fitted to experimental data to give confidence in its validity for scale-up of the design.

Heterogeneous reaction

When a catalyst is used inside a heat-exchange device, the designer faces the same issues as for homogeneous reactions, with the added complication of modifying the exchanger mechanical design to contain the catalyst.

Catalyst can be loaded into the tubes of a shell and tube heat exchanger if the exchanger is mounted vertically and a suitable retaining screen is used at the end of each tube or immediately below the bottom tubesheet. This arrangement is used in the oxidation of orthoxylene to phthallic anhydride, where the reaction is cooled using a circulating molten salt, as illustrated in Fig. 15.25. Heat from the molten salt is used to raise steam.

For high-temperature endothermic reactions, heat input from steam or molten salt is not practical, and the reactor must be designed for heat input from a fired heater. The rate of heat input in the convective section of a heater is usually too low to be useful because of the low heat transfer coefficient of the flue gas, so the reactor tubes must normally be placed in the radiant section of the furnace. It is difficult to maintain a uniform loading of catalyst in a horizontal tube, so the reactor tubes are typically hung vertically. The design must allow for thermal expansion of the tubes, which makes the use of U-tubes difficult, as the cold spot may be in one side of the U, causing the tube to bend. Several ingenious proprietary designs have been developed to overcome this problem. For example, ICI developed a tube-in-tube design for use in the steam reforming of methane to hydrogen, which is illustrated in Fig. 15.26. The chemistry of methane steam reforming is discussed in more detail in Example 4.5. In the ICI design

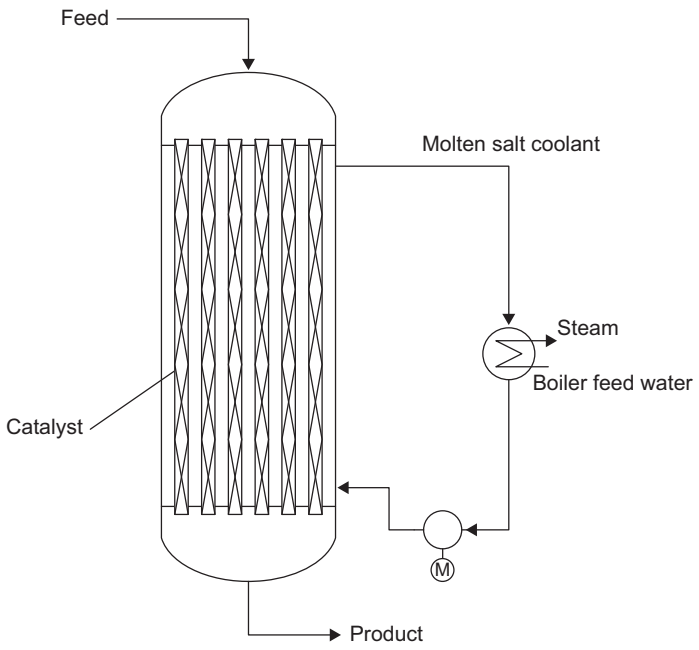


FIG. 15.25 Phthalic anhydride reactor.

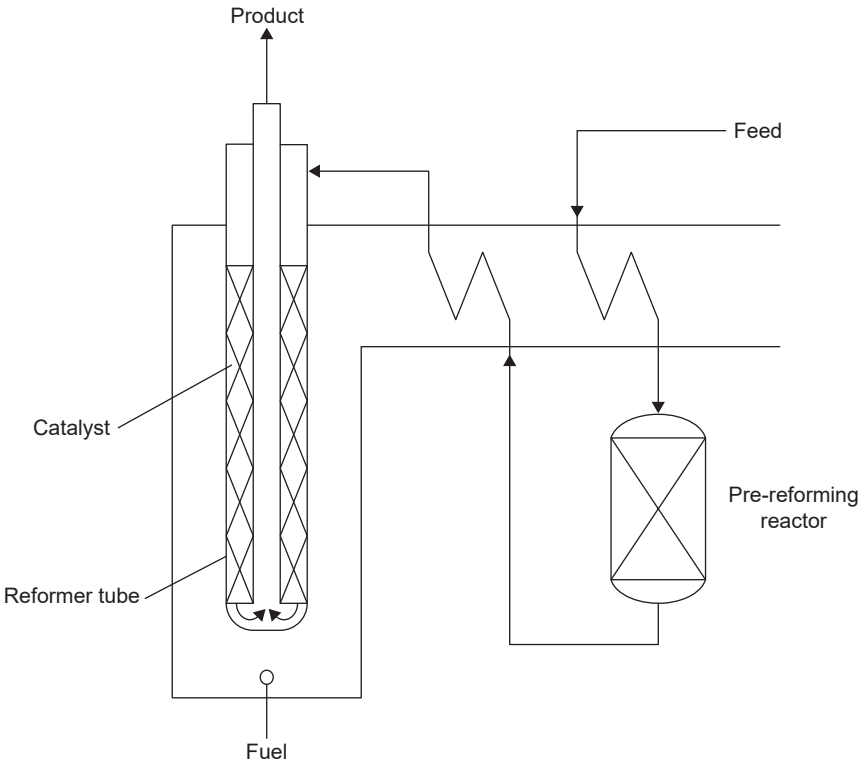


FIG. 15.26 ICI tube-in-tube steam reforming reactor. *From US 4,985,231.*

the feed is pre-heated in the convection section of the furnace, passed through a pre-reforming reactor, and reheated in the convection section before entering the reforming tubes. The reforming tubes have a tube-in-tube arrangement, with catalyst loaded in the annular space. The process gas passes down through the catalyst and then exits through the inner tube. It can be seen that if the inner and outer tubes experience different thermal expansion, there will be no loss of containment of the catalyst or bending of the tubes.

Heat transfer to packed beds of catalyst can be modeled using the equations developed by Leva (1949); see Section 15.3.4. The same cautions apply as for design of homogeneous heat exchanger reactors, and detailed models of the kinetics and hydrodynamics must be used to scale up a design.

15.7 Multiphase reactors

In multiphase reactors, the design is complicated by the need to promote mass transfer between the phases, which is usually accomplished by providing a high interfacial area. If more than one phase is flowing, the design may also need to allow for phase separation.

15.7.1 Vapor–liquid reactors

Vapor–liquid reactions are important in many chemical processes. Many oxygenation and hydrogenation reactions of organic compounds are carried out with the organic component in the liquid phase.

Vapor–liquid contacting columns are preferred for vapor–liquid reactors if the residence time requirements are short enough because of the high area for mass transfer. Packed columns are usually used; see Section 17.14. When long residence time is needed for the liquid phase, stirred tanks or tubular reactors are used. Methods of mixing a gas into a liquid are described in Section 15.5.3, and the mass transfer rates obtained when gas is sparged into a stirred tank can be predicted using Equations 15.13 to 15.15; see Section 15.3.4.

The kinetics of gas–liquid reactions depend on the relative rates of mass transfer and chemical reaction. Consider the case where a gas species A reacts with a liquid species B. If the reaction is second order, the rate of reaction per unit volume can be written as:

$$\Re = k_2 C_A C_B \tag{15.17}$$

where:

C_A = concentration of A in the liquid phase
C_B = concentration of B in the liquid phase
k_2 = second-order rate constant

If component B is present in excess in the liquid, we can assume that its composition is constant, in which case we can rewrite Equation 15.17 as:

$$\Re \approx k_1 C_A \tag{15.18}$$

where:

$k_1 = k_2\, C_B$

Now consider mass transfer of component A through the boundary layer at the vapor–liquid interface, shown schematically in Fig. 15.27.

The rate of mass transfer per unit volume of liquid can be written as:

$$\text{Rate of mass transfer} = k_L a\left(C_{A,i} - C_{A,bulk}\right) \tag{15.19}$$

where:

k_L = mass transfer coefficient for component A in the liquid phase
a = interfacial area per unit volume of liquid
$C_{A,i}$ = concentration of A in the liquid at the interface (as predicted by phase equilibrium)
$C_{A,bulk}$ = concentration of A in the bulk liquid

If most of the reaction occurs in the bulk liquid, then the rate of reaction in the liquid must be equal to the rate of mass transfer through the film, and we can equate Equations 15.18 and 15.19:

$$\mathrm{k_1 C_{A,bulk} = k_L a\left(C_{A,i} - C_{A,bulk}\right)} \tag{15.20}$$

hence:

$$C_{A,bulk} = \frac{k_L a}{(k_1 + k_L a)} C_{A,i} \tag{15.21}$$

and we can rewrite the rate of reaction as:

$$\Re = k_1 C_{A,bulk} = \quad k_L a \;\; C_{A,i} \frac{k_1}{(k_1 + k_L a)} \tag{15.22}$$

Two cases are apparent from Equation 15.22. If $k_L a >> k_1$:

$$\Re \approx k_1 C_{A,i} \tag{15.23}$$

This is known as the slow kinetics–controlled regime, and the reaction occurs at the rate that would be predicted with the liquid-phase concentration predicted by phase equilibrium. In this regime the rate is not sensitive to the interfacial area and increasing the agitation rate or packing area per unit volume will not affect the conversion.

Alternatively, if $k_1 >> k_L a$:

$$\Re \approx k_L a \;\; C_{A,i} \tag{15.24}$$

This is known as the slow mass-transfer–controlled regime, in which the reaction rate is equal to the rate of mass transfer that would be obtained if the concentration of A in the bulk were zero. The rate of reaction is directly proportional to the interfacial area.

If the thickness of the boundary layer is δ, and the condition for either of these regimes is that the reaction rate in the bulk is greater than the reaction rate in the film, we can write the condition as:

$$a\delta \; k_1 C_{A,i} << a k_L \left(C_{A,i} - C_{A,bulk}\right) \tag{15.25}$$

The definition of the mass transfer coefficient is $k_L = D_A/\delta$, and if $C_{A,bulk} \approx 0$, we can derive:

$$\frac{D_A k_1}{k_L^2} << 1 \tag{15.26}$$

or $Ha^2 << 1$, where Ha is the Hatta number:

$$\text{Ha} = \frac{\sqrt{D_A k_1}}{k_L} \tag{15.27}$$

and D_A = diffusion coefficient of A in the liquid phase.

If Ha is roughly equal to or greater than 1.0, then the reaction occurs substantially in the boundary layer and the analysis becomes more complicated. Details of the equations obtained in the resulting regimes can be found in reaction engineering textbooks such as Froment et al. (2010) and Levenspiel (1998).

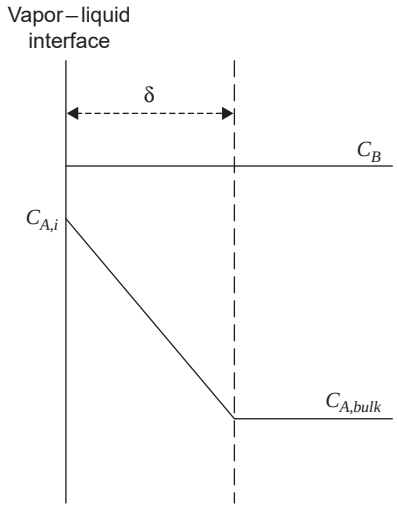


FIG. 15.27 Mass transfer from vapor to liquid.

Many vapor–liquid reactions of commercial significance occur in the slow regimes because oxidation and hydrogenation reactions are exothermic and are usually carried out at low temperature to improve selectivity. The use of falling-film wetted column reactors of known area can allow measurement of k_L and k_1 for use in reactor scale-up. Most gas–liquid reactions are operated under conditions where the gas component is not fully converted so as to ensure that the reaction does not become starved of reagent. Unreacted gas can be recycled (with a purge to prevent buildup of impurities), but inexpensive gases such as air are usually used once through.

15.7.2 Liquid–liquid reactors

Liquid–liquid reactions occur between immiscible liquid phases, usually an organic phase and an aqueous phase. Examples include reactions such as the nitration of toluene or benzene with mixed acids, emulsion polymerizations, and many reactions that are catalyzed by liquid acids, such as motor fuel alkylation.

Liquid–liquid reactions are usually carried out in stirred tank reactors so that agitation can be used to generate a high liquid–liquid area for mass transfer. The reactor is typically followed by a settling tank, similar to the mixer–settler arrangement used for single-stage extraction, so that the phases can be separated for further processing, although settling is usually carried out in the reactor itself in a batch process. The decision of which phase will be continuous and which phase will be dispersed is usually made based on the required hold-up of each phase, ease of dispersing one phase in the other, or safety considerations. In most cases, reaction only occurs in one phase or at the interface between the phases.

The equations used to describe mass transfer with reaction in a liquid–liquid system are analogous to those for vapor–liquid reactions, and the overall rate is often determined by mass transfer rather than the intrinsic kinetics. Mass transfer control of a liquid–liquid reaction can be detected experimentally by varying the agitation rate with other conditions kept constant. When increasing the agitation rate no longer affects the conversion, the reaction is no longer mass transfer controlled and the intrinsic kinetics can be found.

Prediction of liquid–liquid mass transfer rates is difficult due to surfactant effects on droplet coalescence and breakup, and the equations used for vapor–liquid mass transfer coefficient cannot be extrapolated to liquid–liquid systems. Scale-up is usually carried out by finding a condition at which mass transfer is not controlling and then assuming the same agitator power input per unit volume of reactor.

Some examples of liquid–liquid reactor designs are given in the discussion on liquid–liquid heterogeneous catalysis in Section 15.8.2.

The design of settling tanks is relatively straightforward and is discussed in Section 16.4.1.

15.7.3 Vapor–solid reactors

Gas-phase reactions that use solid catalysts can be carried out in fixed, moving or fluidized bed reactors. When a gas reacts with a solid reagent, a fluidized-bed reactor is usually used.

Fixed-bed reactors

In a fixed-bed reactor, the gas flows over a stationary packed bed of catalyst. Fixed-bed catalytic reactors are probably the most common type of reactor for high-temperature catalytic processes and for gas conversion. Examples of processes that use fixed beds include ammonia synthesis, oxidation of sulfur dioxide, isomerization of n-alkanes (paraffins), and the reaction of benzene with ethylene or propylene to form ethylbenzene or cumene.

Fixed-bed reactors can range in size from a few centimeters diameter inside a heat exchanger tube up to several meters diameter for large-scale processes in oil refineries. Reactors greater than 14 ft (4.27 m) are generally avoided because of the need for site fabrication, but if the reactor is to be designed for high-pressure operation, then one larger, site-fabricated vessel may still be cheaper than using two parallel reactors.

In most gas-phase fixed-bed reactors, the gas enters at the top of the reactor and flows down through the bed of catalyst. Up-flow can be used, but the designer must take care to avoid conditions that would cause fluidization; see Section 18.2.2. Distribution of the gas across the bed is easy, as the pressure drop along the bed is much greater than the pressure drop in the head space of the vessel. In some cases, the head space is filled with inert ceramic balls so that catalyst is only loaded to the tangent line of the vessel. A layer of inert ceramic balls is also usually used at the bottom of the reactor to help contain the catalyst (Fig. 15.28).

The outlet of a fixed-bed reactor must be designed with a suitable collector to retain the catalyst and prevent it from being carried out into downstream operations. The outlet collector is usually a can with perforated walls that is welded inside the outlet nozzle.

Fixed-bed reactors can be sized as follows:

1. From the space velocity determine the bed volume of catalyst required.
2. Assume the bed volume is contained in the tangent-to-tangent section of a pressure vessel (not the head space). The vessel will be a cylinder, usually with aspect ratio between 1:1 and 4:1.
3. Check the pressure drop. If pressure drop is too high, then use a lower aspect ratio.
4. If multiple reheats or quenches are needed, make allowance for internals between the beds.
5. Design the pressure vessel using the methods given in Chapter 14.

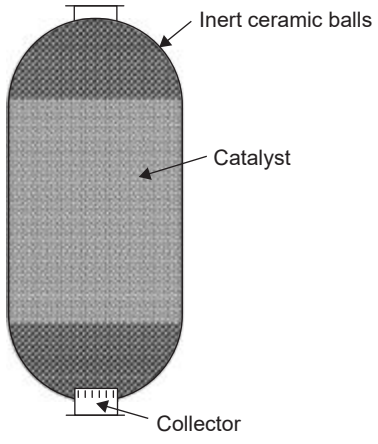


FIG. 15.28 Fixed-bed reactor loading.

The pressure drop in a fixed-bed reactor can be calculated using the Ergun equation (Ergun, 1952):

$$\frac{\Delta P}{L_b} = 150\frac{(1-\varepsilon)^2}{\varepsilon^3}\frac{\mu\ u}{d_p^2} + 1.75\frac{(1-\varepsilon)}{\varepsilon^3}\frac{\rho_f u^2}{d_p} \tag{15.28}$$

where:

ΔP = pressure drop, N/m^2
L_b = length of the bed of solids, m
ε = void fraction
μ = fluid viscosity, Ns/m^2
u = fluid superficial velocity, m/s
d_p = particle effective diameter, m
ρ_f = fluid density, kg/m^3

If there is a constraint on the pressure drop, this will set a limit on the length of the bed and cause the designer to select a vessel with lower aspect ratio. The design of a fixed-bed reactor is illustrated in Example 15.4.

If a very low-pressure drop is required, then instead of designing a "pancake" reactor with very low aspect ratio, a radial-flow packed bed can be used. In a radial-flow reactor the catalyst is contained in an annulus between vertical perforated or slotted screens. The fluid flows radially through the bed, and the direction of flow can be either inwards or outwards. A schematic radial-flow reactor is shown in Fig. 15.29. The use of radial flow allows for a much smaller bed length while maintaining a compact vertical cylindrical pressure vessel.

Packed-bed reactors are normally operated adiabatically, although packed beds can be accommodated inside heat exchanger or furnace tubes. See Section 15.6.3 for a discussion of heat addition and removal from fixed-bed reactors. When a fixed bed of catalyst is divided into smaller beds to allow reheats or quenches, some volume allowance must be made for collection and redistribution of the gas. The vessel design must also allow for the additional nozzles (branches) needed for the flows to and from the heaters or coolers.

Many fixed-bed reactors operate at temperatures substantially above ambient. The design must make allowance for bed settling due to thermal expansion of the vessel. Frequent heating and cooling of fixed-bed reactors should be avoided, as contraction of the vessel during cooling will compress the catalyst and can crush the catalyst, leading to fines formation and pressure-drop problems.

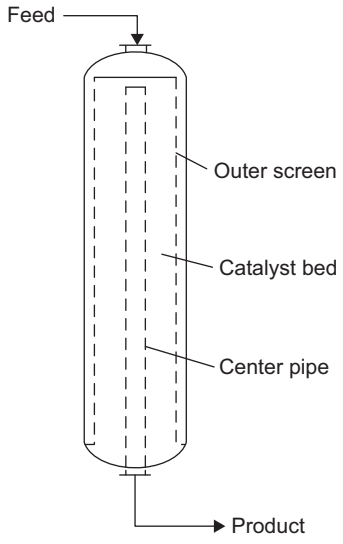


FIG. 15.29 Radial-flow reactor.

Moving-bed reactors

A moving-bed reactor is essentially a fixed-bed reactor that accommodates slow movement of the solids. Moving-bed reactors are used when the solids require gradual change-out—for example, when the catalyst deactivates at a rate that is too rapid for periodic regeneration *in situ* but not rapid enough to warrant the extra cost of using a fluidized-bed system.

Most industrial moving-bed reactors are radial-flow reactors in which the catalyst flows downwards between the retention screens, while the gas flows radially across the moving bed. An example is the UOP CCR Platforming process for catalytic reforming of naphtha, which uses a moving bed to enable catalyst regeneration. Three or four beds in series are used, with reheats between the beds, and the beds are stacked vertically to allow catalyst to flow through all the beds before being sent to a separate regeneration reactor. The design is illustrated in Fig. 15.30, reproduced with permission of UOP, LLC.

Many other proprietary moving-bed reactor designs have been developed, and these can easily be found by searching in patent databases such as www.uspto.gov or www.delphion.com.

The design of a moving-bed reactor must allow for the space needed for catalyst transfer lines, as well as the bed volume and other reactor internals. A detailed mechanical layout of the reactor should be made before sizing the pressure vessel. When evaluating a new design, large-scale, cold-flow models are often built to ensure that the solids flow properly.

Fluidized-bed reactors

In a fluidized-bed reactor the solid particles are fluidized by the gas flow. Several different types of fluidized-bed reactors are possible, corresponding to the different regimes of fluidization. Fluidized-bed reactors are widely used for conversion of solid reagents, for example, in coal combustion, coal gasification, and biomass pyrolysis; for processes that form a solid at high temperature, such as fluidized coking or polymerization; and for catalytic processes where the rate of catalyst deactivation is high and frequent regeneration is needed, as in the catalytic cracking of heavy oils in oil refining.

The physics of fluidization and the properties of fluidized beds are discussed in Section 18.2.2. It can be seen from Fig. 18.8 that fluidization spans a broad range of behavior, from expanded beds through bubbling to spouting and ultimately pneumatic transport. A reaction can be carried out under any of these conditions, leading to a combination of possible mixing patterns, as illustrated in Fig. 15.31.

Near to incipient fluidization the gas flows through the bed with little back-mixing. Although the solid particles are moving, there is no long-range mixing in the solid bed (see Fig. 15.31a). When the gas flow increases, bubbles begin to form. The bubbles agitate the fluidized bed, causing the solids to approach a well-mixed state, while the gas phase remains in plug flow, but with some degree of bypass due to the bubbles (see Fig. 15.31b). In turbulent

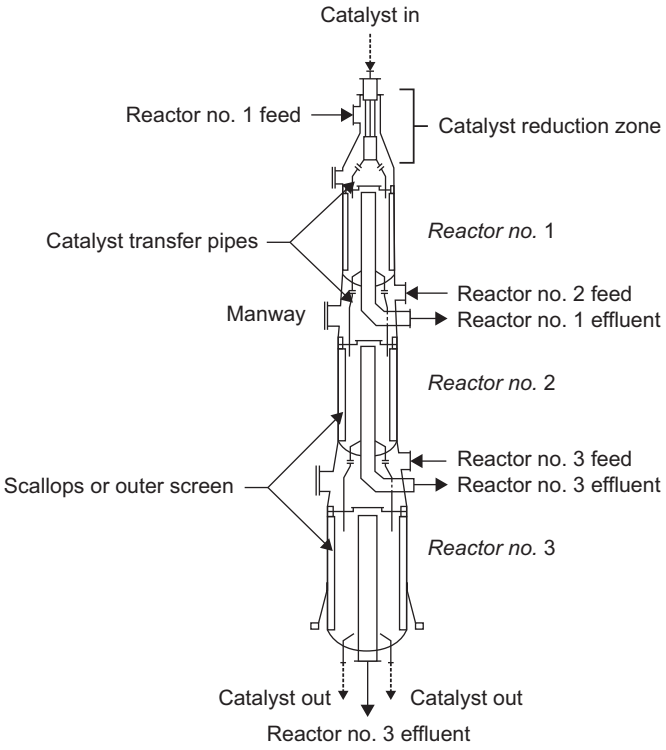


FIG. 15.30 UOP catalytic reforming reactor.

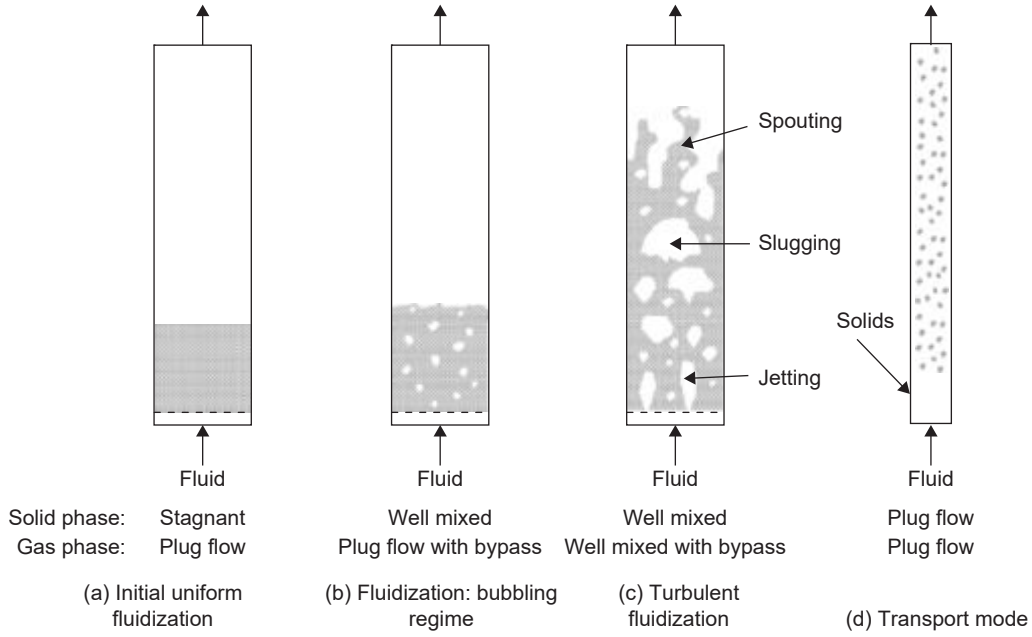


FIG. 15.31 Fluidized-bed reactor modes.

fluidization, the solids are well mixed, and the violent agitation of the bed causes back-mixing of the gas phase, causing it to also approach well-mixed behavior (see Fig. 15.31c). In this regime there can be substantial bypass of the bed by the gas phase due to the presence of jets, spouts, and large bubbles. Finally, when the gas velocity is high enough to entrain the solids, pneumatic conveying occurs and the solids flow with the gas in transport mode, with both phases approximating plug flow (see Fig. 15.31d). Note that in a transport fluidized bed the velocity of the solid particles is not necessarily the same as the velocity of the gas, depending on the flow direction. The slip velocity between the gas and solid particles can be found from a force balance between buoyancy and drag (essentially the same balance used to calculate terminal velocity).

The rates of heat and mass transfer in fluidized beds are much higher than in fixed beds, and external mass transfer is rarely the rate-controlling process. Heat transfer coefficients on the order of 200 $W/m^2\ ^\circ C$ to jackets and internal coils are typically obtained.

Fluidization can only be used with relatively small sized particles: <300 μm with gases. The solid material must be strong enough to withstand attrition in the fluidized bed and cheap enough to allow for make-up to replace attrition losses. The solids may be a catalyst, a reactant in fluidized combustion processes, or an inert powder added to promote heat transfer.

Modeling the kinetics of reactions in fluidized beds can be challenging because of the complex mixing that occurs, the possibility of bypass due to bubbles, and the difficulty of predicting the residence time distributions of the solids and the fluid phase. An introduction to modeling fluid bed reactions is given in Froment et al. (2010); see also Rase (1977), Grace et al. (1996), and Basu (2006). The use of combined models of particle dynamics and kinetics is described in Jung et al. (2009).

In addition to accommodating the expanded fluidized bed of solids, a fluidized-bed reactor must make allowance for separating the gas-phase product from entrained solids so that solids are not carried out of the reactor. This is usually accomplished using one or two stages of cyclones at the reactor exit. The cyclones can be mounted externally to the reactor, or internally, with dip legs that ensure return of solids into the bed, as illustrated in Fig. 15.32. The design of cyclones is described in Section 18.5.3. After bulk solids recovery, methods such as fabric filters or electrostatic precipitation are used for control of fine particulates. These and other processes for recovering residual particles from the reactor product are described in Section 18.5. Any equipment downstream of the particulate control equipment must still be designed for the presence of dust.

Depending on the hardness of the particles and the operating temperature of the reactor, it may be necessary to provide a fluidized-bed reactor with a refractory lining to prevent erosion by the particles.

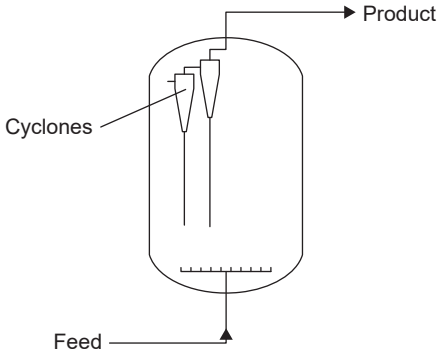


FIG. 15.32 Fluidized-bed reactor with internal cyclones.

15.7.4 Liquid–solid reactors

The reactors used for vapor–solid reactions can all be used for liquid–solid reactions if the liquid is flowing continuously. More care is needed when specifying up-flow of a liquid through a packed bed, as the smaller difference in density between a liquid and a solid increases the buoyancy of the solid and makes fluidization more likely. Down-flow is consequently preferred for packed-bed liquid–solid reactors.

Liquid–solid reactions can also be carried out in a slurry phase, in which the solid is mixed up in the liquid. Slurry reactors are prone to attrition of the solids, caused by pumping or agitation of the liquid. In some processes this attrition is desirable, for example, in reactions that convert solid minerals. In processes where a solid phase is being formed, as in slurry polymerization or reactive crystallization, the shearing or attrition of the solids can be traded off against the particle growth rate to obtain a desired particle size distribution. The formation of slurries is discussed in Section 18.3.5.

Slurry-phase operation is usually not preferred for processes that use heterogeneous catalysts because the catalyst tends to become eroded and can be difficult to recover from the liquid. Packed beds are usually used instead. If well-mixed reactor performance is desired, a packed bed with an effluent recycle can be used, as shown in Fig. 15.33.

15.7.5 Vapor–liquid–solid reactors

A three-phase reactor is required when a gas and liquid react over a solid catalyst, as in amination of alcohols or hydrogenation reactions, such as the saturation of fats or the desulfurization of petroleum fractions. All fermentation processes are three-phase due to the presence of cells as the solid phase and the need to provide oxygen and remove carbon dioxide from the fermentation broth.

Most vapor–liquid–solid reactions are carried out in either a slurry reactor or a trickle-bed reactor. Packed bubble column reactors are more rarely encountered.

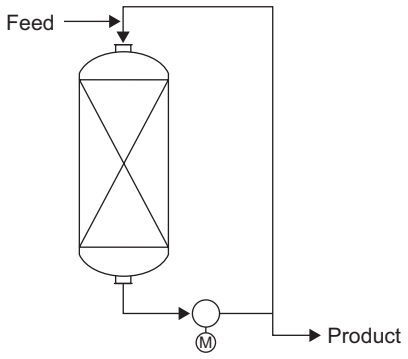


FIG. 15.33 Packed bed with effluent recycle.

Slurry reactors

The use of slurry reactors for liquid–solid reactions was discussed in Section 15.7.4. It is relatively straightforward to bubble or sparge a gas or vapor into a slurry reactor, and the mass transfer rate from gas to liquid can be predicted using the same correlations used for stirred tanks.

At high gas rates, the presence of gas bubbles can help mix the liquid and reduce the need for external agitation. This is exploited in loop reactors and draft-tube reactors. In a loop reactor, the gas is fed at the bottom of one side of a U-shaped reactor loop (the riser) and bubbles up through the liquid. At the top of the riser the gas and liquid disengage. The difference in density between the riser and the other side of the loop creates a hydraulic gradient that causes circulation of the liquid (Fig. 15.34). A draft-tube reactor uses the same concept with the gas fed to a central, cylindrical riser and down-flow occurring in the outer annulus between the draft tube and vessel wall (Fig. 15.35).

When a gas is fed to a slurry reactor, provision must be made for separation of the vapor and liquid in the head space and for recovery of entrained liquid from the exiting gas. If the gas flow is low, droplets will easily settle in the space above the liquid surface and no additional equipment will be needed. If the gas velocity is high, a horizontal settler can be used downstream of the reactor to allow liquid drops to settle and be returned to the reactor. A vent condenser may also be needed if volatile components from the liquid must be recovered. If foaming occurs in the reactor, then the rate of liquid carry-over can be excessive, and an antifoaming agent would typically be added to the reactor.

Trickle-bed reactors

In a trickle-bed reactor the liquid flows down over the surface of a stationary bed of solids. The gas phase usually also flows downwards with the liquid, but countercurrent flow is feasible as long as flooding conditions are avoided. The surface area provided by the solid helps promote vapor–liquid mass transfer, and both the liquid and vapor phase have little back-mixing and approximate plug flow behavior. Examples of processes that use trickle-bed reactors include the hydrocracking of heavy oils and reactions over immobilized organisms in gel columns.

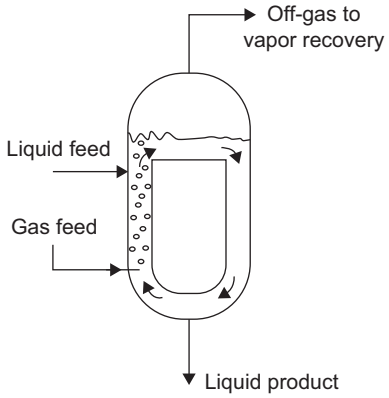


FIG. 15.34 Loop reactor.

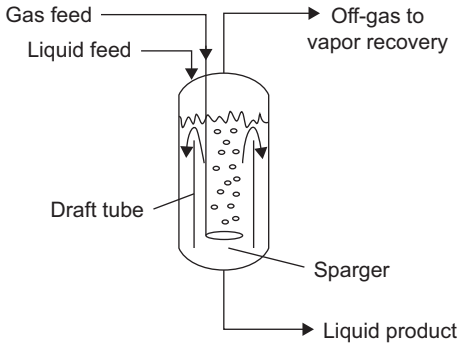


FIG. 15.35 Draft-tube reactor.

One of the most important design aspects of a trickle bed is to ensure proper wetting of the solids. If channeling of the liquid occurs, regions of the bed can be flooded and experience poor vapor–liquid contacting, whereas other regions may have no liquid present at all. Maldistribution of liquid can also cause local hot or cold spots in the reactor, which can affect selectivity and be a safety concern if the reaction is exothermic. Good wetting is particularly difficult to ensure if the heat of reaction causes a significant fraction of the liquid to vaporize as it passes down the catalyst bed or if the reaction forms compounds that vaporize under reaction conditions. The distributors that are used to ensure good liquid coverage of the solids are similar to those used in packed columns; see Section 17.14.5. The reactor designer must make allowance for the space needed for these internals.

Most trickle-bed reactors operate adiabatically. If reheats or quenches are needed between stages, the vapor and liquid must be collected and redistributed onto the stage below.

The pressure drop in a trickle bed is higher than predicted by the Ergun equation; see Al-Dahhan and Dudukovic (1994).

Modeling the kinetics and hydraulics of trickle flow is not trivial. Trickle-bed reactors can be sized following the same method as packed-bed reactors if the space velocity is known from pilot plant data, but prediction of performance from kinetics measured in laboratory-scale slurry reactors is challenging. More information on modeling the performance of trickle-bed reactors is given in the books by Harriott (2002) and Ranade et al. (2011).

15.8 Reactor design for catalytic processes

Most nonbiological industrial reactions are carried out in the presence of a catalyst. If a catalyst can be found that selectively promotes the desired reaction, it will have the following benefits:

- Improved selectivity for the desired product relative to by-products
- Operation at a lower temperature, giving improved selectivity relative to thermal reactions
- Faster rate of reaction, leading to a smaller, less costly reactor

Catalysts are classified as homogeneous if they are in the same phase as the reagents and heterogeneous if they are in a different phase. Most industrial catalytic processes use solid catalysts, as they are easier to contain, handle, and recover, but solid catalysts are more susceptible to poisoning by feed contaminants and to deactivation by accumulation of material inside the pores of the catalyst.

A wide range of materials can serve as catalysts. Some catalysts, such as liquid sulfuric acid, are inexpensive and can be treated as a consumable, with little attempt made to recover the catalyst when it is spent. At the other end of the cost spectrum, many reactions use catalysts that contain noble metals such as platinum and palladium. The value of a reactor load of noble metal catalyst can be several million dollars, and the design must guarantee that catalyst is properly contained and not lost from the system.

When a catalyst is specified, the reactor design must ensure that catalyst activity is maintained and that the catalyst is recovered for reuse, regeneration, or safe disposal. Other specific requirements for different types of catalyst are discussed in the following sections.

15.8.1 Design for homogeneous catalysis

A homogeneous catalyst is a catalyst that is in the same phase as the reagents. Homogeneous catalysts are relatively common in the process industries, but are not preferred because of the difficulty and expense of recovering the catalyst from the reaction mixture. Homogeneous catalysts are most often used in the liquid phase. Some examples include water-soluble enzymes, the use of organometallic compounds of cobalt in oxidation processes, and the use of sodium hydroxide as catalyst in the transesterification of triglycerides with methanol to produce fatty acid methyl esters (FAME, commonly known as biodiesel).

A homogeneous catalyst must either be cheap enough to be used once through in the process and not recovered or else chemically stable enough to withstand the conditions of a downstream recovery process. Salts or metal–ligand complexes can often be recovered from reaction products relatively easily by extraction or by causing the reaction products to separate into two liquid phases. If the product is volatile relative to the catalyst and solvent and the catalyst is thermally stable, it may be possible to flash or distill off the product, leaving a catalyst-rich residue that can be recycled.

Some homogeneous catalysts can be converted into heterogeneous catalysts by immobilizing the catalytic species on the surface or in the pores of a solid. For example, a wide variety of methods have been developed for immobilization of enzymes; see Storey and Schafhauser-Smith (1994). This approach is not always feasible, particularly when the active catalytic species is soluble in the reaction mixture and will leach from the support.

From a safety perspective, an important class of homogeneously catalyzed reactions is autocatalytic reactions. In an autocatalytic reaction, a product or reaction intermediate catalyzes the reaction and increases the reaction rate. Examples include many nitration reactions, reactions that involve peroxides that form hydroperoxide radicals, and other free radical reactions where free radical branching mechanisms can occur. Autocatalytic reactions have the potential to run away and are therefore a serious safety concern. Great care is needed in design and scale-up to ensure that the reaction is controllable, particularly when the reaction is exothermic or is not easily quenched by the addition of a free radical inhibitor. If an alternative, safer route cannot be found, the designer should apply inherently safer design principles to minimize the hazard; see Section 15.13. The design must consider reaction runaway as a relief scenario and as a scenario during hazard and operability (HAZOP) studies.

15.8.2 Design for heterogeneous catalysis

Heterogeneous catalysis is usually preferred over homogeneous catalysis, as it is much easier to recover and reuse the catalyst if it is in a different phase from the reagents. Examples of heterogeneous catalysis can be found in all possible phase combinations, but in the process industries the most common situations are liquid–liquid catalysis and fluid–solid catalysis.

Liquid–liquid catalysis

Reactions that are catalyzed by a different liquid phase include reactions where the catalyst is dissolved or suspended in water and the reagents are in the organic phase, as in the Asahi process for adipic acid by hydration of cyclohexene, and reactions that use liquid acids as catalysts, such as the reactions of alkenes with benzene and the alkylation of isobutane with alkenes to form alkylate for use as a gasoline blend stock. An emerging area of liquid–liquid catalysis is the use of ionic liquids as catalysts. Ionic liquids are salts with very low melting points that are liquid at ambient conditions. Ionic liquids have very low volatility, and variation of the anion and cation can allow optimization of their properties as solvents. Ionic liquids have been proposed as a means of immobilizing transition metal salts as catalysts and, in some cases, as catalysts in their own right; see Stark and Seddon (2007) for multiple examples.

In most liquid–liquid catalytic reactions the reaction occurs at the interface or in one phase only. Surfactant effects can be important, as surfactant molecules can stabilize micelles (or reverse micelles) and have a significant effect on interfacial area. It is not necessary for any of the reagents to be soluble in the catalyst phase to any great extent.

The design of reactors for liquid–liquid catalysis is the same as the design of liquid–liquid reactors; see Section 15.7.2. Mixer–settler reactors are most common, although extraction column reactors can also be used. In a mixer–settler arrangement, the stirred tank is usually operated at a high rate of agitation to maximize the interfacial area.

Several proprietary mixer–settler designs have been developed for liquid–liquid catalyzed processes. For example, isobutane can be alkylated with 2-butene to form 2,2,4-trimethylpentane (iso-octane), as shown in Fig. 15.36. This reaction is important in oil refining, as it allows C_4 compounds that would be too volatile for use in fuels to be converted into a high-octane gasoline blendstock. The reaction is exothermic and is catalyzed by strong acids such as sulfuric acid and hydrofluoric acid.

In the reactor design developed by Stratco (currently licensed by DuPont) and shown in Fig. 15.37, the reaction takes place in an agitated horizontal contacting vessel. The agitator mixes the sulfuric acid and organic phases and causes a circulation over heat-exchange tubes that contain refrigerant. A second vessel is mounted above the reactor and serves as a separator, allowing the organic product to be drawn off and acid to be returned to the reactor.

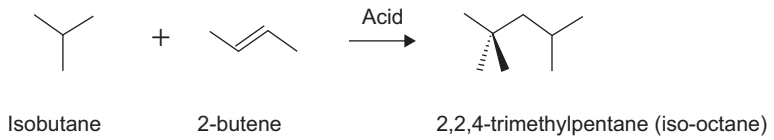


FIG. 15.36 Alkylation of isobutane with 2-butene.

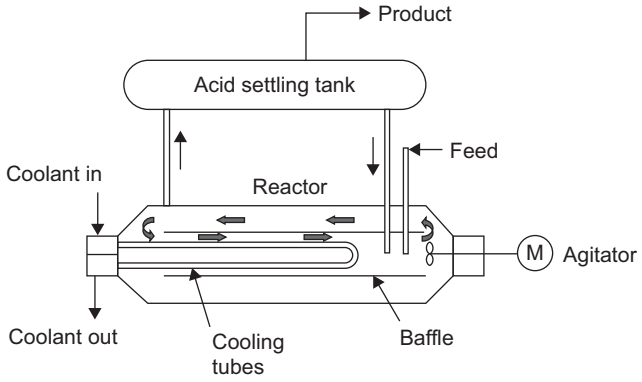


FIG. 15.37 Stratco sulfuric acid alkylation reactor.

An alternative sulfuric acid alkylation reactor design, developed by ExxonMobil, is illustrated in Fig. 15.38. The ExxonMobil design uses auto-refrigeration instead of indirect heat transfer to remove the heat of reaction. Part of the isobutane is boiled off from the reactor, compressed, condensed, and returned to the reactor to provide the necessary cooling. The ExxonMobil reactor has a series of agitated cells with staged feed addition and approximates plug flow with staged feed. The acid and hydrocarbon phases are separated in a separate vessel, and acid is returned to the first reactor cell.

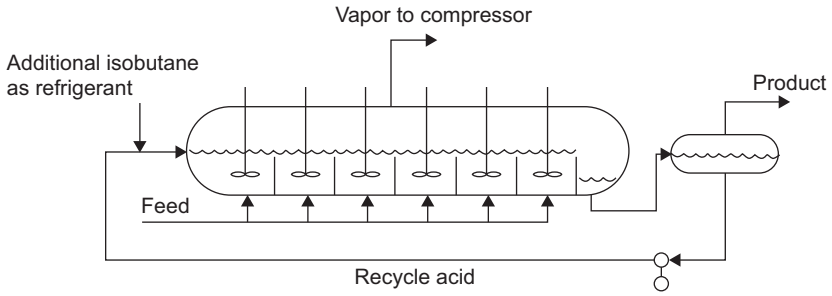


FIG. 15.38 ExxonMobil sulfuric acid alkylation reactor.

Fluid–solid catalysis

In most catalytic processes the catalyst is in a solid form and the reagents are a gas, liquid, or vapor–liquid mixture. The use of solid-phase catalysts is preferred because the separation of a solid from a fluid allows relatively easy recovery and reuse of the catalyst, but solid catalysts have many other advantages that come from the chemical and physical structure of the solid; these are discussed in Section 15.8.3.

The kinetics of a reaction in a porous solid catalyst can be complex, as there are multiple steps to the reaction:

1. External mass transfer of the reagents from the bulk fluid to the catalyst surface.
2. Internal mass transfer of reagents through macropores within the catalyst. Most catalysts consist of smaller particles or crystallites stuck together with a binder (Fig. 15.39). The macroporosity comes from the spaces between crystallites.
3. Internal mass transfer of reagents within micropores or within the crystals themselves.
4. Adsorption of reagents onto the active site on the catalyst surface.
5. Reaction.
6. Desorption of products from the catalyst surface.
7. Internal mass transfer of products within micropores.
8. Internal mass transfer of products through macropores.
9. External mass transfer of products through the boundary layer to the bulk fluid.

Any of these steps can be rate limiting. Multiple mechanisms can be written for adsorption, as well as for the chemical reaction step, so a large number of possible rate equations can be developed for solid catalyzed reactions.

The development of these equations is described in all of the reaction engineering textbooks listed in the bibliography at the end of this chapter. It is often difficult to discriminate between alternative mechanisms, and a given mechanism may be valid over a very narrow range of process conditions. Care must be taken to ensure that rate expressions are developed under conditions that match the conditions expected in a plant reactor; see Section 15.3.3.

Solid catalysts can be used in any of the reactor designs introduced in Section 15.7. Packed-bed reactors are most common, as they minimize the reactor volume required to contain the catalyst, but slurry reactors, moving-bed reactors, trickle-bed reactors, and fluidized-bed reactors are all widely used for catalytic processes.

Solid catalysts can become deactivated by a variety of mechanisms. Some catalysts deactivate slowly over many years, whereas other catalysts can lose their activity in a few seconds. The mechanisms of deactivation and design approaches to catalyst deactivation and regeneration are discussed in Section 15.8.4.

15.8.3 Design and selection of solid catalysts

The process design engineer will very rarely need to design the catalyst for use in the process; catalyst design will usually be carried out by research chemists in a catalyst manufacturing company. It is nonetheless important to understand how catalysts are formulated and manufactured to be able to select the best catalyst for a process application.

Structure and formulation of catalysts

Most solid catalysts are composite materials. In a typical catalyst the active material is either dispersed on the surface of a highly porous support or intermingled with a porous material so as to create a high internal surface area for adsorption and reaction and high porosity for good mass transfer. Some materials such as natural and synthetic zeolites have an open crystalline lattice with channels that are large enough for organic molecules to diffuse inside the crystal. The shape and size of these pores can be exploited to make highly selective catalysts. Many aluminosilicate and aluminophosphate materials have zeolite structures. Varying the ratio of aluminum to silicon or substituting metals into the lattice of these crystals allows adjustment of the Brönsted or Lewis acidity and further increases the options for catalysis. Many examples of zeolite catalysts are given in the books by Breck (1974) and Kulprathipanja (2010).

The manufacture of catalysts usually involves the following steps:

1. Synthesis of small crystals of the active crystalline component.
2. Ion exchange to adjust the acidity.
3. Blending of the active component with support material and binder to form a paste or sol. The function of the binder is to hold the crystallites together (see Fig. 15.39). Clays are usually used as binders, but any material can be used that will form a bond between the crystals without reducing the surface area or adversely affecting chemical or physical properties of the finished catalyst.
4. Forming of the mixture into particles of the desired shape and size. The most common method of forming is to extrude a paste through a die and form a shaped extrudate catalyst. A range of shapes can be formed, as illustrated in Fig. 15.40, but cylinders are most common. Small spherical catalysts are made by spray drying, whereas larger spheres can be made by oil dropping or granulation methods; see Section 18.8.
5. Drying and calcining of the particles. Drying is carried out to remove any residual solvent used in the mixing process. Calcining the catalyst at higher temperature causes the particles to harden and ensures that the formed shape is retained.
6. Impregnation with metals. In many catalysts the active sites are small crystallites or even individual atoms of metal dispersed on the catalyst surface. Metals are usually loaded by wet impregnation methods, in which the catalyst is soaked in a solution of a thermally unstable metal salt and the metal salt is subsequently decomposed at high temperature to leave the metal on the catalyst surface in a reduced form.

The sequence of steps can vary, and some catalysts may not require all of these steps. The resulting catalyst pellets should have an open internal structure that offers a high active surface area for reaction.

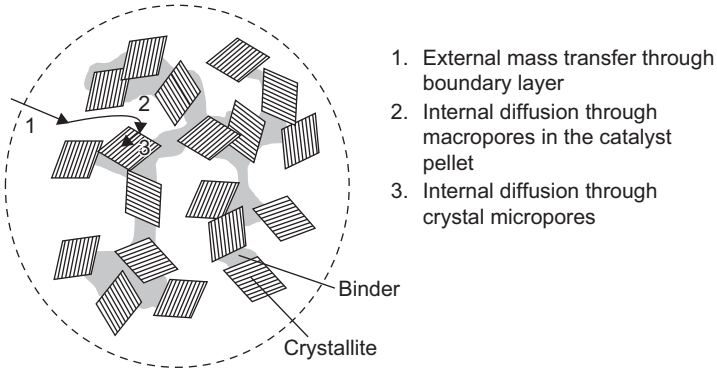


FIG. 15.39 Diffusion steps in a microcrystalline porous solid catalyst.

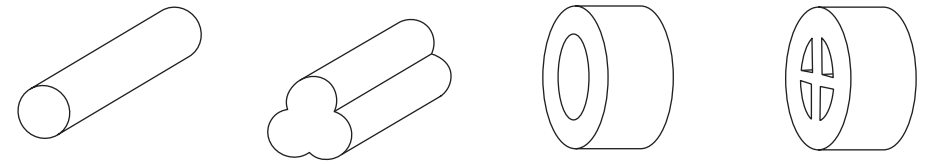


FIG. 15.40 Extruded catalyst shapes.

Physical properties of catalysts

The reactor design engineer must pay attention to some of the physical properties of the catalyst, as well as its chemical effectiveness. The following properties can affect reactor design and performance:

- **Shape**: Extruded catalyst shapes, such as those shown in Fig. 15.40, have higher external surface area per unit volume, which can reduce external mass transfer and heat transfer limitations. Spherical catalysts are preferred in applications where the catalyst is moving, such as slurry, fluidized-bed, or moving-bed reactors. If catalysts with sharp edges are used in these reactors, they will become rounded due to erosion. Part of the catalyst will be lost as fines, and there may be problems with dust carrying into downstream equipment.
- **Size**: Smaller catalyst particles have lower external mass transfer resistance but higher pressure drop when used in a packed bed. Smaller particles are harder to recover from slurries. Fluidized-bed reactors require particles to be in a certain size range to give the desired fluidization behavior; see Section 18.2.2.
- **Composition**: Aside from the active component of the catalyst, the composition of other materials used in the formulation can affect the catalyst properties. If a binder is used, it must be inert under all the expected process conditions, including catalyst regeneration conditions.
- **Porosity**: The external macroporosity of a catalyst formulation can be important in some processes. If the active catalyst has low porosity, then it is usually dispersed onto the surface of a more porous support material to increase the available surface area while retaining a large enough particle for convenient solids handling.
- **Strength**: The catalyst must be strong enough to withstand impacts and attrition that occur during loading and reactor operation. The strength of particulate materials is discussed in Section 18.2. Catalysts are usually composite materials, and the strength can be strongly affected by the choice and amount of binder used.
- **Thermal stability**: Many catalyst supports and catalytically active materials are sensitive to loss of internal surface area by sintering at high temperature. Reaction with steam at high temperature can similarly cause hydrothermal damage. Some catalysts, such as the ultra-stable Y zeolite used in catalytic cracking reactors, retain adequate porosity and activity to still be used after multiple exposures to high temperature. When testing such catalysts, it is important to age the catalyst properly so that the performance reflects the performance the catalyst will have after it has experienced several regenerations.

The characterization and properties of granular solids are discussed in more detail in Section 18.2.

Catalyst testing and selection

Usually several catalyst vendors can provide suitable catalyst for use in a given process application. Catalysts are normally selected based on performance rather than price, as the cost of the catalyst is typically a small fraction of

process operating costs, and a catalyst that has better selectivity will almost always quickly pay back any price premium expected by the manufacturer.

Because the rate-limiting step of the reaction is sensitive to several aspects of the catalyst formulation, it is important to test the catalyst under conditions that are representative of process conditions. Pilot plants can be used if they are benchmarked against full-scale plants and if they properly simulate the effect of recycles, feed contaminants, etc. See Section 15.12.1 for further discussion of experimental validation of reactor performance.

15.8.4 Design for catalyst deactivation and regeneration

Catalysts in process service can lose their activity over time. In some cases, deactivation can be reversed and the catalyst performance can be restored, whereas other deactivation mechanisms are permanent and require the operator to replace the catalyst load. If the design engineer expects that deactivation cannot be avoided, the reactor design must account for catalyst regeneration or replacement.

Catalyst deactivation mechanisms

Catalyst deactivation may be reversible or irreversible. Some of the more common methods of catalyst deactivation and the design methods that are used to prevent them from occurring are described in Table 15.7.

Reactor design for catalyst deactivation

Some of the strategies that are used to prevent catalyst deactivation are listed in Table 15.7. If the rate of deactivation of the catalyst is slow, it is also possible to design the reactor to tolerate a certain extent of deactivation. The two strategies that are most often used are temperature ramping and use of excess catalyst.

In a temperature-ramping strategy, the fresh catalyst is operated at a temperature that is below the maximum temperature recommended for the reaction. As the catalyst activity declines, the operators slowly raise the reactor temperature to maintain the same conversion across the reactor. The operators continue increasing temperature until a temperature is reached at which the reaction selectivity is compromised or the rate of catalyst deactivation is accelerated, at which point it becomes necessary to shut down and regenerate or replace the catalyst. The amount of temperature ramp that can be tolerated is usually recommended by the catalyst vendor. Typical values are 20 to 40 °C over a period that can range from days to several years. When a temperature-ramping strategy is planned, it is important to understand the reactor performance and yields under both start-of-run and end-of-run conditions, as changes in selectivity can occur, creating a need for the designer to examine the impact on downstream equipment.

If excess catalyst is loaded in the reactor, then some of the catalyst can become deactivated without overall performance declining. The use of excess catalyst is limited to reactions where the selectivity at the reactor outlet is insensitive to the amount of catalyst present, for example, processes that approach equilibrium or processes that can afford to overshoot the required conversion. An example of such a process is the hydrodesulfurization of petroleum fractions, where excess sulfur removal exceeds process requirements but does not usually cause significant financial loss.

Reactor design for catalyst regeneration

Catalysts that have become deactivated by coke formation can usually be reactivated by burning off the coke under controlled conditions. The frequency of regeneration required depends on the rate of coke formation. Some catalysts are regenerated after a few years or months of operation, whereas the catalysts used in fluid catalytic cracking of gas oils are regenerated after a few seconds on stream and experience multiple regenerations per hour.

When catalyst regeneration is infrequent, there is usually no need to make special modifications to the reactor design. If the process can afford to be shut down for a period for catalyst regeneration, the regeneration can sometimes be carried out *in situ* in the reactor. In this case, the ancillary equipment needed for regeneration must be added to the process flowsheet. Ancillary equipment may include such items as an air blower, air pre-heater, dust control equipment, etc. More often, the catalyst is unloaded and sent off-site for regeneration. In the meantime, a different batch of catalyst is loaded, allowing the plant to come back on stream faster.

If an interruption in process operation is not acceptable, a cyclic or swing-bed regeneration approach can be used. In cyclic designs, the plant has several reactors and is designed so that one reactor can be taken off-stream for regeneration without affecting the operation of the other reactors. Cyclic regeneration can occur as often as several times an hour, but longer cycles are preferred because they cause fewer thermal cycles and reduce the likelihood of fatigue damage. Cyclic regeneration designs need particular attention to the selection of the switching valves that are used

TABLE 15.7 Catalyst deactivation mechanisms

Mechanism	Causes	Design approaches to mitigate deactivation
Reversible poisoning	Feed components or contaminants that adsorb reversibly on the catalyst active site. Common reversible poisons include ammonia, arsine, phosphine, water, hydrogen sulfide, oxygen, and carbon monoxide.	If the feed concentration of a reversible poison is higher than the design basis value, the effect can often be reversed by returning to the design level. Upstream separation processes can be used to remove contaminants. Guard beds of adsorbent can also be used.
Irreversible poisoning	Contaminants that are strongly adsorbed on the catalyst or react irreversibly with the active site. Examples include sulfur dioxide and halogens, although water and ammonia can irreversibly damage strong acid catalysts.	If the presence of irreversible poisons is expected, then a guard bed of adsorbent should be placed upstream of the reactor. See Section 16.2.1 for design of adsorption processes. Irreversible adsorbents are usually used to ensure a strong interaction that will tie up the contaminant. A sacrificial bed of low-activity catalyst at the inlet of the reactor can also be used as a mitigation technique.
Amalgamation	If mercury is present in a feed, it can amalgamate with metals on the catalyst and destroy the metal function.	Guard beds containing copper- or silver-based adsorbents are used to protect catalysts from mercury.
Coking	Accumulation of carbon-rich deposits on the catalyst. Coke is usually formed by condensation reactions between unsaturated organic compounds. Coke can cover the active sites or block the pores that lead to them.	The effect of coking can usually be reversed by burning off the coke. Care must be taken to ensure that the conditions during coke burn do not lead to deactivation by other mechanisms.
Sintering and hydrothermal damage	Sintering is caused by exposure to high temperatures; hydrothermal damage occurs when high temperatures are combined with concentrations of steam. The effect of both is a reduction in internal surface area, and in some cases loss of crystallinity. Thermal damage of enzyme-based catalysts can occur at relatively low temperatures.	Sintering and hydrothermal damage are prevented by avoiding the conditions under which they can occur. Particular care is needed during catalyst regeneration. Regeneration is often carried out using depleted air that has been enriched in nitrogen or using a recycle of flue gas, so as to limit the temperature rise and the concentration of water that occurs. Thermal damage of enzyme-based catalysts is avoided by using cooling and temperature control to keep the temperature in the desired range.
Agglomeration	Metals on the catalyst can become agglomerated instead of dispersed over the surface, reducing the number of available active sites. Agglomeration can be accelerated by tramp metals that find their way onto the catalyst from the feed or from corrosion products.	In some cases it may be possible to redisperse the metals during a regeneration process, as occurs in catalytic reforming, where some agglomeration of the noble metals on the catalyst occurs during regeneration and a chlorination step is used to redisperse the metal; however, agglomeration is often irreversible.
Leaching	Metals on the catalyst or immobilized catalysts such as enzymes become dissolved in the process fluid and are elutriated from the reactor.	Leaching is irreversible, and the design should try to avoid conditions that can cause it to occur.
Fouling and plugging	Materials such as dust, catalyst fines, corrosion products, gums, dirt, etc., can be filtered by a fixed bed, causing the bed or reactor internals to become plugged and leading to an unacceptable increase in pressure drop.	Filters can be used upstream of the reactor to remove material that can cause plugging. In packed beds, a layer of highly porous inert ceramic material is sometimes placed on top of the catalyst to trap out plugging agents. A periodic back-flush can sometimes reverse the effects of plugging.

to isolate the process conditions from the regeneration conditions, and these valves can be a substantial component of the reactor section cost.

Several commercially important processes make use of continuous catalyst regeneration. If the rate of catalyst deactivation is fast, continuous regeneration offers several advantages relative to cyclic regeneration:

- The process can be operated under conditions where deactivation is more rapid, as regeneration can be more frequent.
- The catalyst maintains optimum activity and selectivity in the reactor, leading to a less costly reactor and better process performance.
- Maintenance and reliability problems due to the switching valves are eliminated.
- Thermal cycling of vessels is eliminated, reducing stresses on vessels and supports.
- Catalyst damage due to stresses on the catalyst bed from thermal cycling is eliminated.
- Regeneration equipment is smaller and operates more efficiently in continuous mode.

Continuous regeneration designs use at least two reactors: one for the process reaction and one for regeneration. Catalyst circulates between the process reactor and the regeneration reactor. Many variations are possible, and some designs have multiple reactors, either in parallel or in series, connected to the same regenerator. Examples of different proprietary reactor–regenerator designs can be found in the patent literature at www.uspto.gov.

Moderate rates of coke formation can be addressed by use of a moving-bed continuous catalyst regeneration design. In a moving-bed reactor the catalyst is slowly circulated between the reactor and regenerator, and the residence time can vary from a few hours to a few days in each zone. A simplified schematic diagram of a moving-bed continuous regeneration design is shown in Fig. 15.41. The proprietary designs used commercially are substantially more complex and can involve several regeneration zones and multiple reactors, with reheats of the process fluid between reactors.

Care must be taken to ensure separation between the hydrocarbon-rich atmosphere of the reactor and the oxygen-rich atmosphere of the regenerator. In moving-bed regeneration systems, inert gas purges or lock hoppers can be integrated into the catalyst lift and transfer system to ensure that a flammable mixture is not formed.

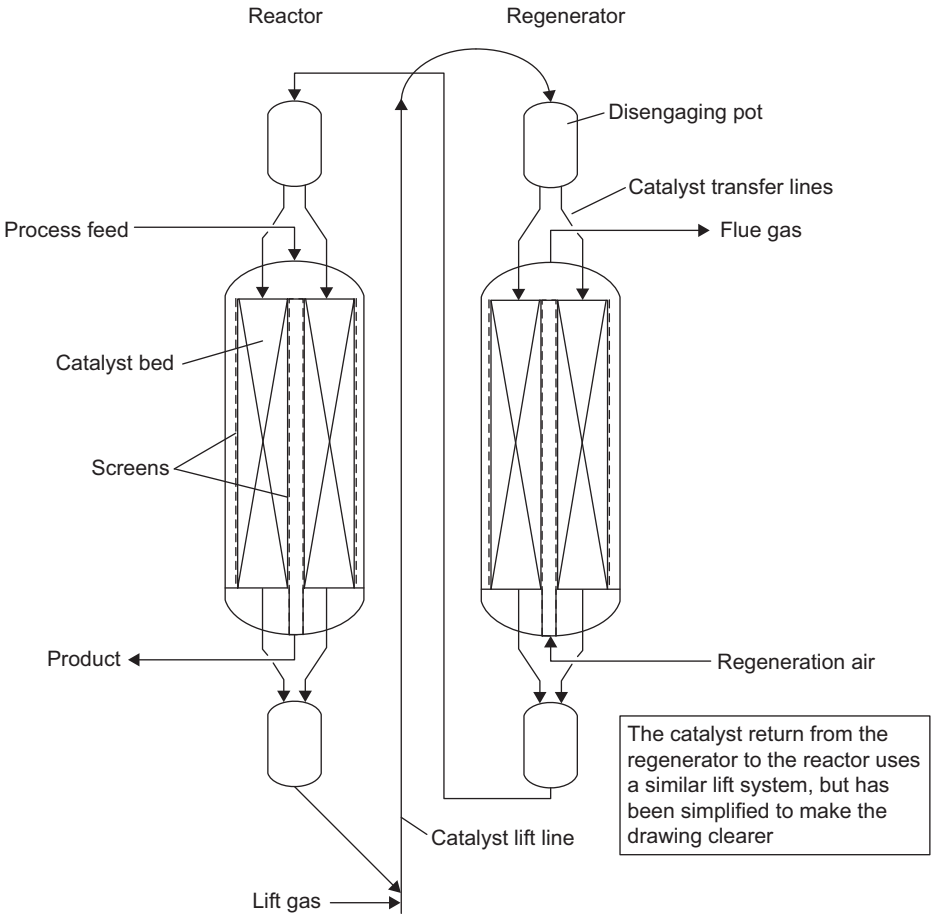


FIG. 15.41 Simplified schematic of a moving-bed reactor system for continuous catalyst regeneration.

In a moving-bed reactor, the catalyst flows as a packed bed moving under gravity, and the catalyst is only fluidized during pneumatic transport in the lift lines between the vessels (see Fig. 15.41). Radial-flow reactors are often used, as they give a more uniform catalyst residence time than moving packed beds. The hydraulic design of moving-bed reactors can be complex, and the designer must ensure that the design allows for controlled flow of the solids as well as process fluids.

Moving-bed reactors are most commonly applied to gas–solid reactions, although they can also be used for liquid–solid reactions. Moving-bed reactors allow flow of solids without the high rates of attrition that are encountered in slurries and fluidized beds, and are therefore attractive when the catalyst is expensive or prone to attrition. Moving-bed reactors are used in the catalytic reforming of naphtha and the catalytic dehydrogenation of propane to propylene. For more details on these processes, see Meyers (2016).

At high rates of coke formation, slow movement of the catalyst is no longer feasible. Instead, very high rates of catalyst circulation can be achieved by using fluidized-bed reactors for both reaction and regeneration and transferring fluidized catalyst between the reactor and regenerator. This approach is used in the FCC of gas oils to lighter hydrocarbons in oil refining.

A catalytic cracking reactor–regenerator system is illustrated in Fig. 15.42, which is reproduced with permission of UOP, LLC. In catalytic cracking, hot regenerated catalyst enters the bottom of a transport riser reactor. The catalyst is fluidized using steam as lift medium and flows up the riser. Gas oil feed is sprayed onto the catalyst, where a variety of cracking reactions occur, forming lighter hydrocarbon products that can be used to make petrochemicals and transportation fuels such as gasoline and diesel. At the top of the riser the solids are separated from the reaction mixture using cyclones, and the reactor product is sent to a fractionation section for product recovery. The catalyst from the top of the riser is stripped with steam to recover hydrocarbons and then passes through a stand pipe to the regenerator. In the regenerator, coke that formed in the reactor is burned off the catalyst, restoring the catalyst activity so that the catalyst can be returned to the riser reactor. The heat from burning the coke is used to vaporize the gas oil feed and to provide the heat needed to give the desired riser reactor outlet temperature.

Over 350 FCC units are in operation worldwide, and almost a quarter of the world's oil production is processed through catalytic cracking. Many different proprietary designs of FCC reactors and regenerators have been developed and can be found in the patent literature; see www.uspto.gov. Catalyst residence times in the riser are typically a few seconds, but can be as short as fractions of a second. The rate of catalyst circulation is typically between five and ten times the feed rate on a mass basis, and large catalytic cracking reactors can have catalyst circulation rates as high as 1.6 metric tons per second. More information on FCC is given in Meyers (2016).

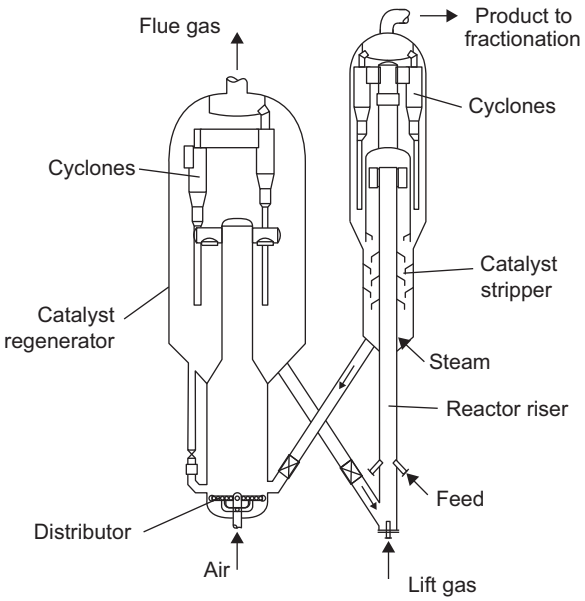


FIG. 15.42 UOP fluidized catalytic cracking reactor and regenerator.

Example 15.4

A new process is being developed for converting benzene to cyclohexane by hydrogenation over a noble metal catalyst. The reaction is carried out at 50 bara, at a feed temperature of 220 °C, and the reactor contents should not exceed 300 °C to minimize formation of methylcyclopentane (MCP) by-product. The reaction is essentially irreversible under these conditions, and the temperature can be controlled by staged addition of cold hydrogen. Six beds are to be used, each converting the same amount of benzene, with overall conversion of 100%. The average weight hourly space velocity based on benzene is 10 h^{-1} for each adiabatic bed, and a pressure drop of 0.5 bar is acceptable across each bed. The catalyst is in the form of 1/16 in (1.588 mm) beads with average bulk density of 700 kg/m^3. Design, size, and cost a reactor for making 200,000 metric tons per year of cyclohexane using this process.

Cautionary note: This example is hypothetical, and all numbers in the problem statement are fictitious. Any resemblance to any commercial cyclohexane technology is purely coincidental.

Solution

The first step is to determine the flow rates around the reactor. Assuming 8000 hours operation per year, the product rate is 200,000/8000 = 25 t/h. To make 1 kg of cyclohexane (C_6H_{12}) requires 78/84 = 0.929 kg of benzene (C_6H_6), so the plant feed rate is 0.929 × 25 = 23.2 t/h.

The hydrogen quench rates must be calculated from a heat balance at process conditions. These calculations are most easily performed using a commercial process simulation program.

Fig. 15.43 shows a screen shot of a reactor model built using UniSim Design R390. Six conversion reactors were used, with the specified conversion of benzene adjusted to give the same amount of benzene converted in each (i.e., 16.7% conversion in

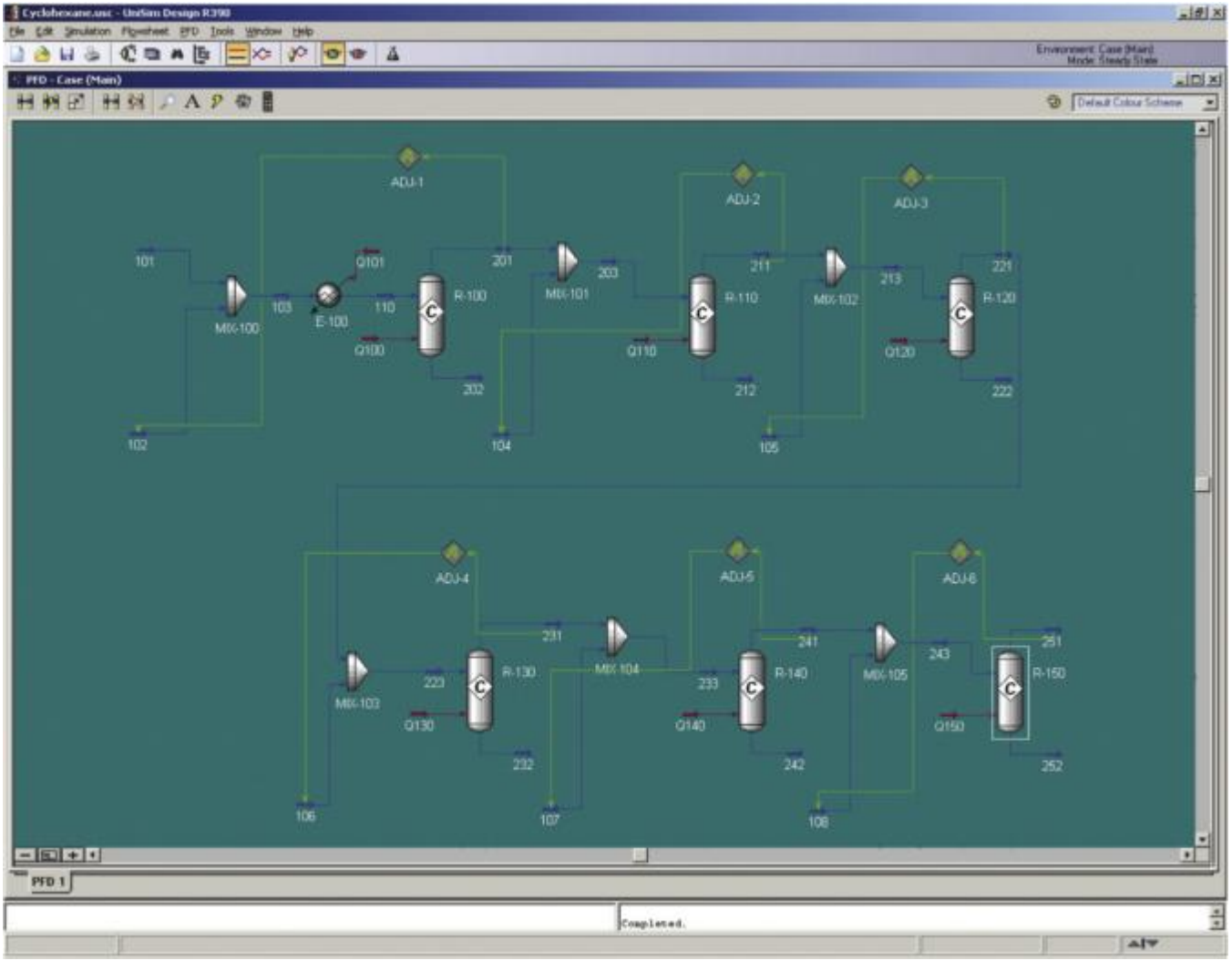


FIG. 15.43 UniSim Design model of cyclohexane reactor for Example 15.4.

TABLE 15.8 Stream flows and properties for Example 15.4

Bed	R100	R110	R120	R130	R140	R150
Inlet temperature (°C)	220	239	251	259	264	269
Outlet temperature (°C)	300	300	300	300	300	300
Feed flow (kmol/h)	3445	4781	6065	7403	8744	10030
Feed flow (kg/h)	29546	32539	35427	38424	41426	44320
Feed flow (act. m^3/h)	2860	4172	5465	6843	8254	9642
Product flow (act. m^3/h)	3214	4566	5892	7299	8738	10151
Feed density (kg/m^3)	10.33	7.80	6.48	5.61	5.02	4.60
Product density (kg/m^3)	9.19	7.13	6.01	5.26	4.74	4.37
Feed viscosity (Ns/m^2)	1.62E-05	1.59E-05	1.57E-05	1.57E-05	1.56E-05	1.56E-05
Product viscosity (Ns/m^2)	1.87E-05	1.77E-05	1.72E-05	1.69E-05	1.66E-05	1.65E-05

R100, 20% in R110, 25% in R120, 33.3% in R130, 50% in R140, and 100% in R150). Adjust controllers were used to set the interbed quench hydrogen flow rate so that the reactor outlet temperature was 300 °C on each reactor. The heat duty to each reactor was specified as zero. A pressure drop of 0.5 bar was allowed on each reactor. From the simulation, we can download the necessary stream flows and properties, which are given in Table 15.8.

Next we must calculate the bed volume to get an idea of what bed diameters will be suitable. With a feed rate of 23,200 kg/h of benzene and WHSV of 10 h^{-1}, the mass of catalyst in each bed is 23,200/10 = 2320 kg. Because the catalyst has average bed density 700 kg/m^3, catalyst bed volume = 2320/700 = 3.314 m^3.

For a given column diameter we can now calculate the bed cross-sectional area and length of bed. In addition to the height required for the catalyst, we must leave some allowance for the hydrogen inlet piping and quench zone between beds. Examining the hydrogen quench flow rates, this will need at least 8-in piping, so a 3-ft (0.914-m) height allowance should be made between beds. For example:

If bed diameter = 6ft = $6 \times 0.3048 = 1.829$ m
Bed cross-sectional area = $\pi D_b^2/4 = 3.142 \times (1.829)^2/4 = 2.627$ m^2
Bed length for 3.314 m^3 bed volume = 3.314/2.627 = 1.262 m
Length of catalyst bed plus quench zone = 1.262 + 0.914 = 2.176 m
Total reactor length for six beds, noting that we only need five quench zones = $6 \times 2.176 - 0.914 = 12.142$ m. We also need some space for a bottom support grid, say 0.30 5m, so total length = 12.447 m.
Vessel aspect ratio = length/diameter = 12.447/1.829 = 6.8

This calculation is easily coded in a spreadsheet and repeated for other bed diameters, giving the results in Table 15.9.

Using the actual volume flow and cross-sectional area, we can now estimate the superficial velocity, and hence use the Ergun equation (Equation 15.28) to estimate the pressure drop. It can be seen from Table 15.8 that the increase in temperature across the reactor has a stronger effect on density than the decrease in molar flow rate due to reaction, so the outlet conditions govern the pressure drop. We could attempt to break each bed into sections to get a more accurate estimate of pressure drop,

TABLE 15.9 Bed and reactor dimensions for Example 15.4

Diameter (ft)	6	7	8
Diameter (m)	1.83	2.13	2.44
Area (m^2)	2.63	3.58	4.67
Bed length (m)	1.262	0.93	0.71
Quench zone length (m)	0.914	0.91	0.91
Tangent length (m)	12.446	10.438	9.135
Aspect ratio (L/D)	6.8	4.9	3.7

but a conservative simplifying assumption is to just use the outlet condition. For example, for R150 (the final bed), with bed diameter 1.829 m:

Reactor outlet actual volume flow = 10,151 m^3/h
Superficial velocity = $10151/(2.627 \times 3600) = 1.073$ m/s

From Table 15.8, at the bed outlet, the density is 4.37 kg/m^3 and the viscosity is 1.65×10^{-5} Ns/m^2. The bed void fraction is not given, but 0.4 is a reasonable value for beads, so substituting in Equation 15.28:

$$\frac{\Delta P}{L_b} = 150\frac{(1-\varepsilon)^2}{\varepsilon^3}\frac{\mu\ u}{d_p^2} + 1.75\frac{(1-\varepsilon)}{\varepsilon^3}\frac{\rho_f u^2}{d_p} \tag{15.28}$$

$$\frac{\Delta P}{1.262} = 150\frac{(1-0.4)^2}{0.4^3}\frac{1.65\times10^{-5}\times1.073}{0.001588^2} + 1.75\frac{(1-0.4)}{0.4^3}\frac{4.37\times1.073^2}{0.001588}$$

$$\text{hence: } \Delta P = 73027\ \text{N/m}^2 \approx 0.73\ \text{bar}$$

In this case the pressure drop is higher than the allowable 0.5 bar, and a larger bed diameter should be considered. This calculation is easily coded into a spreadsheet and repeated for different diameters, giving the results in Table 15.10.

From Table 15.10, either a 7-ft or 8-ft reactor would have an acceptable pressure drop across all the beds. We have not made any allowance for pressure drop in the quench zone, so if we assume this will need ~0.25 bar, then the 8-ft vessel should be selected.

We can now make an estimate of the required wall thickness.

Design pressure, take as 10% above operating gauge pressure:

$$= (50-1)\times 1.1 = 53.9\ \text{bar}$$

$$= 5.39\ \text{N/mm}^2$$

Maximum operating temperature is 300 °C (572 °F). With a 50 °F design margin, design temperature = 622 °F.

From Table 14.2, if we select a 1¼ Cr steel such as A387, the maximum allowable stress = 16.6×10^3 psi = 114.5 N/mm^2. Assuming full radiographic examination, the welded joint efficiency is 1.0, so we can substitute in Equation 14.13:

$$t = \frac{P_i\, D_i}{2SE - 1.2\, P_i} \tag{14.13}$$

$$t = \frac{5.39 \times 2.44 \times 10^3}{(2 \times 114.5 \times 1) - (1.2 \times 5.39)} = 59.1\ \text{mm} \tag{14.13}$$

$$\text{add corrosion allowance} \quad 59.1 + 3 = 62.1\ \text{mm}$$

So the wall thickness is 61 mm, or roughly a 2.5-in plate.

Under these conditions of temperature and pressure, it is probably worth specifying a hemispherical head, so the head thickness can be found using Equation 14.17:

$$t = \frac{P_i\, D_i}{4SE - 0.4P_i} \tag{14.17}$$

$$t = \frac{5.39 \times 2.44 \times 10^3}{(4 \times 114.5 \times 1) - (0.4 \times 5.39)} = 28.9\ \text{mm} \tag{14.17}$$

So with a corrosion allowance, the head thickness needed is 32 mm, or 1¼ in.

TABLE 15.10 Bed pressure drop as a function of reactor diameter for Example 15.4

Bed	R100	R110	R120	R130	R140	R150
Pressure drop (bar): 6 ft	0.165	0.253	0.349	0.464	0.592	0.730
Pressure drop (bar): 7 ft	0.069	0.105	0.145	0.192	0.244	0.300
Pressure drop (bar): 8 ft	0.033	0.050	0.068	0.090	0.114	0.140

Knowing the vessel wall thickness and dimensions, we could now calculate the shell weight and use Equation 7.9, together with the correlation in Table 7.2, to obtain an estimate of the reactor cost; however, a more accurate approach is to use a commercial cost estimating program, such as Aspen Capital Cost Estimator. Fig. 15.44 shows the data entered into ACCE. This gives a total vessel cost of $\underline{\underline{\$697,600}}$ on a January 2006 basis.

The final step in completing the design would be to work with a mechanical engineer to prepare a scale design drawing for detailed mechanical design of the vessel and internals. A preliminary sketch for such a design is shown in Fig. 15.45, but there are many details still missing, such as the location of thermowells for temperature control, support brackets for internals and vessel skirt, design of the quench zone, etc.

Example 15.5

An alternative process for converting benzene to cyclohexane also uses a supported noble metal catalyst, but carries out the reaction in the liquid phase, at a temperature of 160 °C and pressure of 100 bara, in a slurry reactor. The catalyst has piece density 1100 kg/m^3. Laboratory-scale experiments in an isothermal, continuous well-mixed reactor, cooled in a bath of coolant, have determined that with a high rate of hydrogen agitation and 10wt% loading of catalyst, a conversion of 95% can be attained with 40 minutes' residence time.

To scale up this reaction, it is proposed to operate a slurry reactor, agitated by hydrogen, at 95% conversion and to recycle unconverted benzene. Design and size a reactor for making 200,000 metric tons per year of cyclohexane using this process.

Cautionary note: This example is hypothetical and all numbers in the problem statement are fictitious. Any resemblance to any commercial cyclohexane technology is purely coincidental.

Solution

The first step is to estimate stream flow rates and properties and determine the rate of heat removal. These calculations can easily be carried out using a commercial process simulation program.

Fig. 15.46 shows a simulation model of the slurry reactor. The conversion is known, so a conversion reactor can be used. The hydrogen feed can be set in ratio to the benzene feed using a "Set" controller. The hydrogen feed must be in excess of the stoichiometric requirement to provide agitation, so it is reasonable to assume that we will need to recover evaporated liquid from the hydrogen off-gas. Returning this cold liquid as a recycle to the reactor feed reduces the reactor heat duty. We can then use an "Adjust" controller to manipulate the benzene feed rate to give the desired cyclohexane product rate.

Because the reactor temperature was specified, in the simulation model the reactor outlet stream temperatures are specified, and the heat duties will then be calculated by the simulation.

A quick examination of the stream data for the flow scheme in Fig. 15.46 reveals two things:

- The liquid recycle in stream 207 contains 90.9 mol% cyclohexane, whereas the liquid product in stream 202 is only 87 mol% cyclohexane. As might be expected, the condensate is enriched in the lighter product.
- The duty of the condenser, Q102, is 688 kW, whereas the duty of the reactor, Q100, is 14,480 kW.

It is therefore immediately apparent that a recycle of condensate makes very little sense. We would be recycling a product-rich stream, thereby potentially losing selectivity, and the sensible heat required to heat the recycle back to reaction temperature would be only a fraction of the heat of condensation, which itself is less than 5% of the total cooling duty. We can therefore simplify the flow scheme by eliminating the condensate recycle.

Fig. 15.47 shows a revised simulation model without recycle of condensate. The condensate stream is now recovered into the product. The hydrogen flow rate was arbitrarily set at 110% of stoichiometric to ensure that sufficient hydrogen would be available for agitation. The results of this simulation are given in Table 15.11 and can be used as stream data for sizing the reactor.

From Table 15.11, reactor liquid feed (stream 101) volume flow rate = 28.4 m^3/h

Reactor residence time = 40 minutes; therefore liquid volume in reactor = $28.4 \times 40/60 = 18.93$ m^3

We also need to add the volume for the catalyst in the slurry. The liquid density in the reactor is the same as that of the reactor liquid product (stream 202), that is, 624.5 kg/m^3, so:

Mass of liquid in reactor = $624.5 \times 18.93 = 11824$ kg

Mass of catalyst in reactor = 10% of total = $11824/9 = 1314$ kg

Volume occupied by catalyst = $1314/1100 = 1.19$ m^3

Total reactor volume occupied by slurry = $1.19 + 18.93 = \underline{\underline{20.13 \text{ m}^3}}$

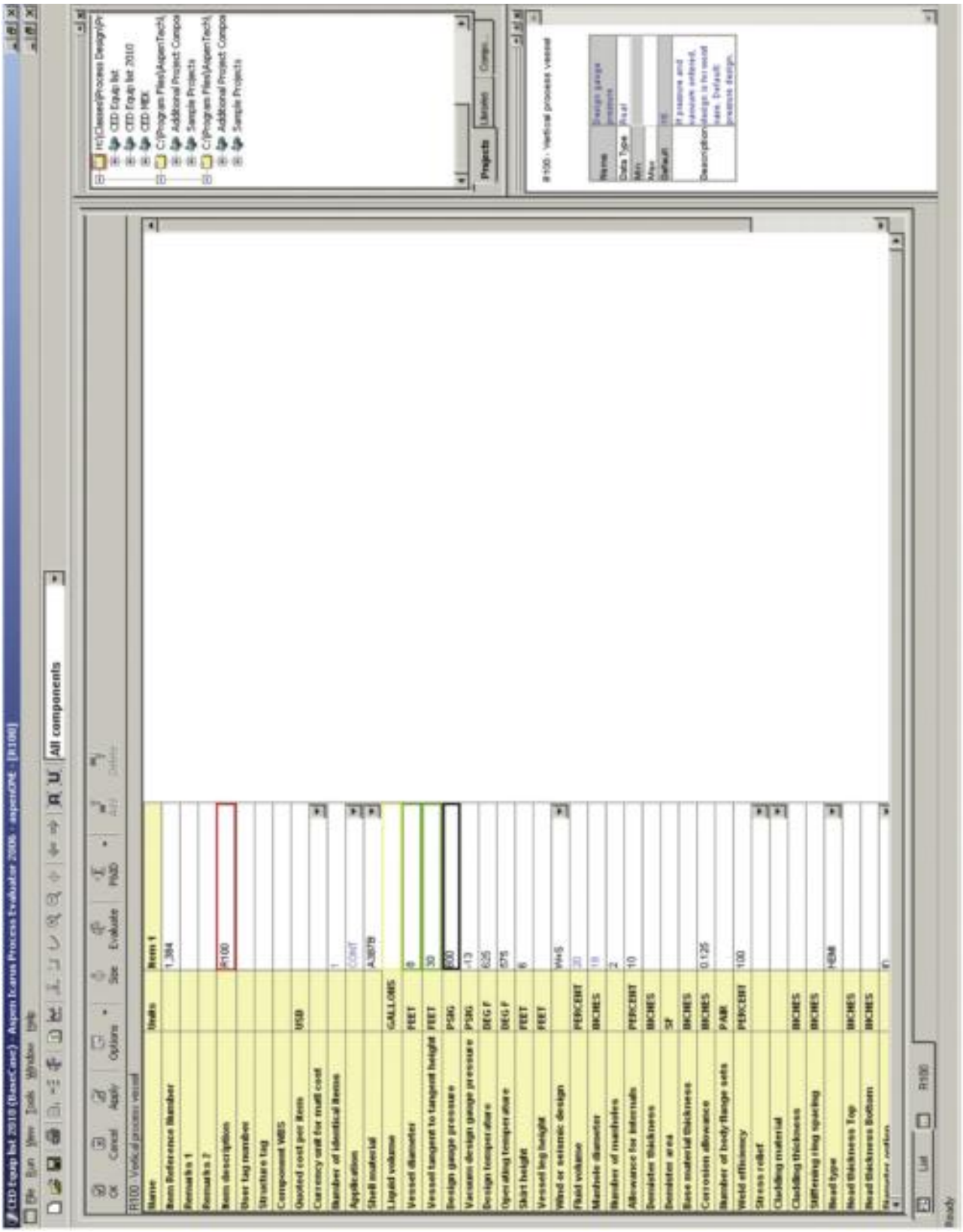


FIG. 15.44 Aspen ICARUS data entry for Example 15.4.

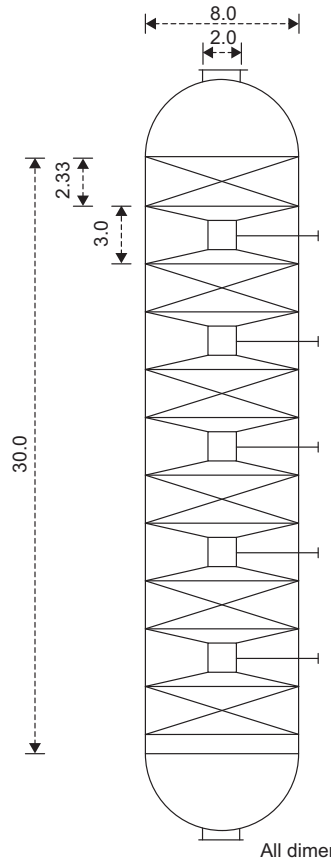


FIG. 15.45 Preliminary reactor design for Example 15.4.

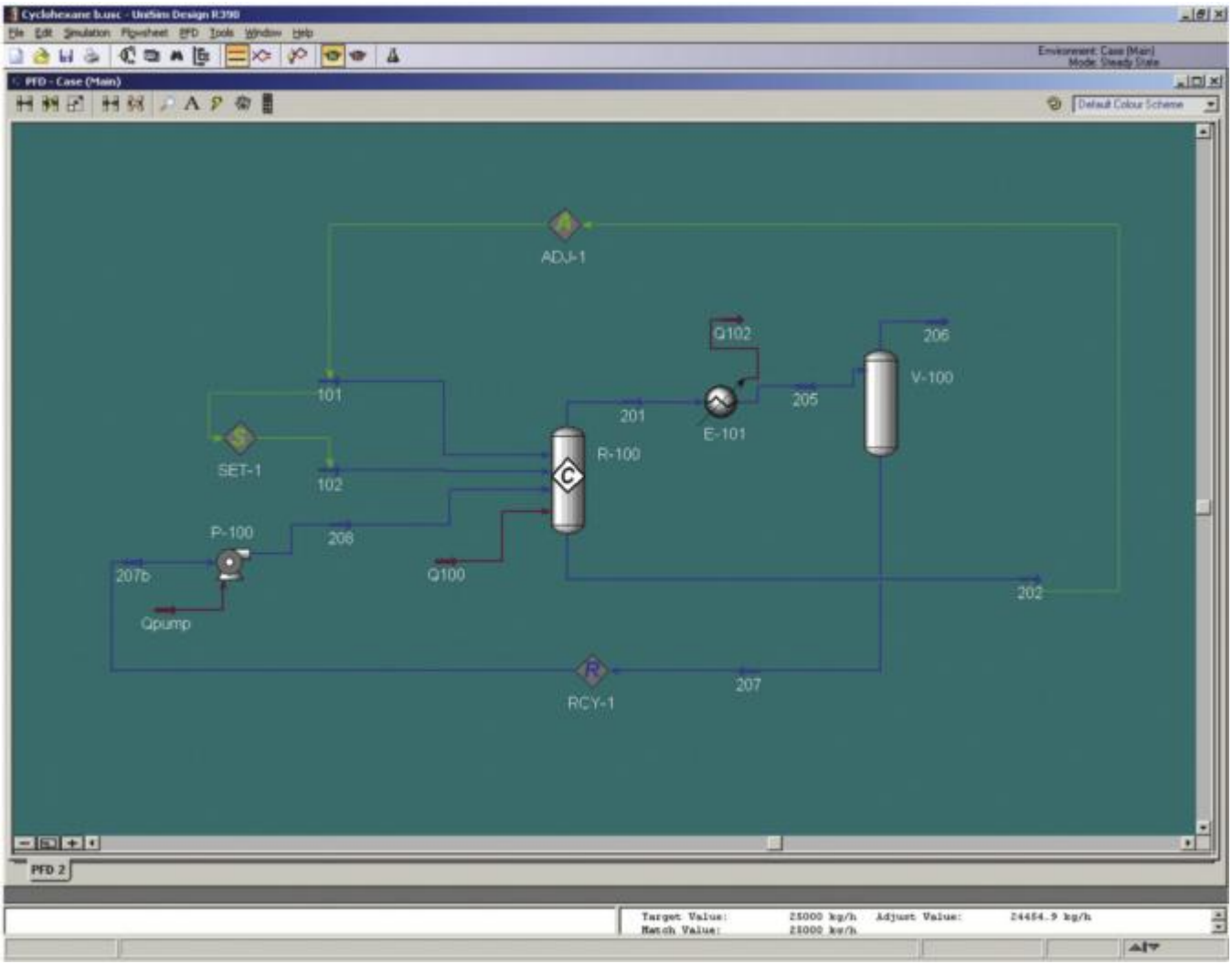


FIG. 15.46 UniSim Design model of cyclohexane slurry reactor with condensate recycle.

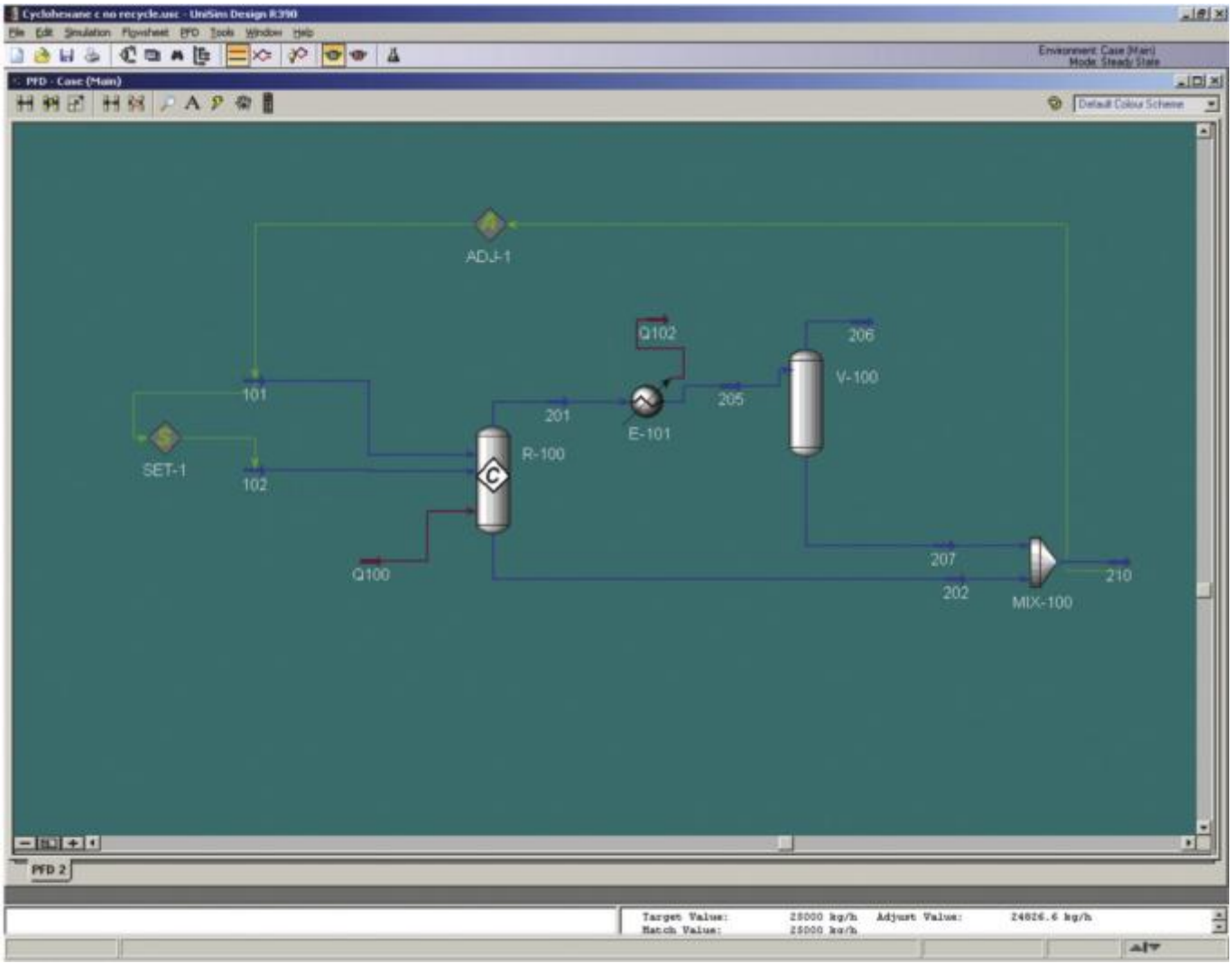


FIG. 15.47 UniSim Design model of cyclohexane slurry reactor.

TABLE 15.11 Simulation results for Example 15.5

Stream	101 Liq feed	102 Gas feed	201 Gas Product	202 Liq Product	205 Cooled Gas	206 Net gas	207 Condensate	210 Product
Vapor fraction	0	1	1	0	0.9069	1	0	0.0003
Temperature (C)	40	40	160	160	50	50	50	156.6
Pressure (kPa)	10020	10020	10000	10000	9980	9980	9980	9980
Molar flow rates (kmol/h)								
Benzene	313.31	0.00	0.63	15.04	0.63	0.03	0.59	15.63
Hydrogen	0.00	1033.93	114.30	26.69	114.30	113.78	0.53	27.21
Cyclohexane	0.00	0.00	11.22	286.43	11.22	0.59	10.62	297.05
Total	313.31	1033.93	126.15	328.16	126.15	114.41	11.74	339.90
Mass flow rates (kg/h)								
Benzene	24472.8	0.0	49.0	1174.6	49.0	2.7	46.4	1221.0
Hydrogen	0.0	2084.4	230.4	53.8	230.4	229.4	1.1	54.9
Cyclohexane	0.0	0.0	943.9	24106.0	943.9	49.9	894.0	25000.0
Total	24472.8	2084.4	1223.4	25334.5	1223.4	282.0	941.4	26275.8

TABLE 15.11 Simulation results for Example 15.5—cont'd

Stream	101 Liq feed	102 Gas feed	201 Gas Product	202 Liq Product	205 Cooled Gas	206 Net gas	207 Condensate	210 Product
Properties								
Mass density (kg/m^3)	862.1	7.5	26.3	624.5	36.8	8.8	751.1	628.3
Act. volume flow (m^3/h)	28.4	278.9	46.5	40.6	33.2	32.0	1.3	41.8
Mass heat capacity (kJ/kg-C)	1.57	14.40	4.37	2.51	4.17	11.99	1.83	2.49
Thermal conductivity (W/m-K)	0.127	0.188	0.181	0.082		0.189	0.114	
Viscosity (cP)	0.498	9.40E-03	1.59E-02	0.1523		9.65E-03	0.5616	

TABLE 15.12 Gas superficial velocity as a function of diameter for Example 15.5

Diameter (ft)	Area (ft^2)	Gas flow top (ft/min)	Gas flow bottom (ft/min)
4	12.57	2.18	13.06
5	19.64	1.39	8.36
6	28.28	0.97	5.81
7	38.49	0.71	4.27
8	50.27	0.54	3.27
9	63.63	0.43	2.58
10	78.55	0.35	2.09

We can now try different reactor geometries that could accommodate this volume. Because the reactor is agitated using hydrogen, it is important to understand the extent of agitation, and hence the gas superficial velocity. The gas actual volume flow at the bottom and top of the reactor can be read from Table 15.11 as the actual flow rates of streams 102 and 201. These can be used to calculate the superficial velocity at the top and bottom of the reactor assuming a cylindrical geometry. The results are shown in Table 15.12, in units of ft/min, so as to be consistent with the velocities specified in Table 15.6.

From Table 15.6, we would ideally prefer the gas velocity to be in the range of 1 to 3 ft/min. The change in gas flow rate due to the reaction is large enough that no diameter gives an ideal velocity at both ends. The diameters above 7 ft appear to give velocities that are a bit low at the outlet, whereas 4 ft and 5 ft may be a bit high at the bottom, so it looks like 6 ft is about right.

For a 6-ft (1.829-m)−diameter cylindrical vessel, cross-sectional area $= \pi\ (1.829)^2/4 = 2.627$ m^2
Height for 20.13 m^3 volume $= 20.13/2.627 = 11.00$ m or 36 ft

It is not clear that a vessel 36 ft tall by 6 ft diameter would be well mixed by bubbling gas through it. A better design might be to use a draft tube reactor, with the hydrogen flow driving liquid circulation, as discussed in Section 15.7.5 and illustrated in Fig. 15.35. The slurry volume is then set by the outer diameter. If we choose an outer diameter of 10 ft (3.048 m), then:

For a 10-ft-diameter cylindrical vessel, cross-sectional area $= \pi\ (3.048)^2/4 = 7.298$ m^2
Height for 20.13 m^3 volume $= 20.13/7.298 = 2.76$ m or 9 ft

Note that this is the height of the section filled with liquid, and we will require some additional space above the liquid. We also need to make some allowance for the gas hold-up (i.e., the void space filled by bubbles).

The next thing to consider is the required heat removal. From the simulation model, the reactor cooling duty is 14.94 MW, at isothermal temperature of 160 °C. If boiling water is used as coolant (for constant temperature and high heat transfer coefficient), then low-pressure steam could be raised at 2 bar, 120 °C, giving a 40 °C temperature difference. A quick estimate of the overall heat transfer coefficient can be made from Fig. 19.1. If the process side is a light organic and utility side is boiling water, then an overall heat transfer coefficient of about 650 W/m^{2}K is reasonable. The area can then be estimated using Equation 19.1:

$$Q = UA\Delta T_m \tag{19.1}$$

where : Q = heat transferred per unit time, W
U = the overall heat transfer coefficient, W/m$^{2^\circ}$C
A = heat transfer area, m^2
ΔT_m = the mean temperature difference, the temperature driving force, °C

$$\text{Substituting} : 14.94 \times 10^6 = 650 \times A \times 40$$

$$\text{Required area} = 14.94 \times 10^6/(650 \times 40) = 574.6 \text{ m}^2$$

This is quite a large area and obviously too large to use a cooling jacket or coil. We can investigate how many tubes would be needed if we used a stab-in heat exchange bundle:

$$\text{Area of 1-inch diameter tube, 9 ft long} = \pi \times 0.0254 \times 2.76 = 0.220 \text{ m}^2$$

$$\text{Number of tubes required for heat transfer (if bundle is inside reactor)} = 574.6/0.22 = 2612$$

Such a large number of tubes would clearly not be easy to accommodate inside the draft tube without a significant effect on hydraulics. Instead, we must consider an external exchanger. If we choose to pump liquid from the reactor, cool it with cooling water to 60 °C (allowing a 20 °C approach so that a cross-flow exchanger with a X-shell can be used to minimize fouling or blocking by catalyst fines), and then return it to the reactor, then a heat balance gives the required flow rate:

$$\text{Specific heat capacity} = \text{heat capacity of stream 202} = 2.52 \text{ kJ/kg}^{\circ}\text{C}$$

$$\text{Mass flow rate} = 14.94 \times 10^6/(2.52 \times 10^3 \times 100) = 54.05 \text{ kg/s} = 194.6 \text{ t/h}, \text{ or roughly 7.6 times the product rate.}$$

This is not unacceptably high, given that we have 11824 kg of liquid in the reactor, but the pump-around loop must circulate the entire reactor contents every $11824/(54 \times 60) = 3.6$ minutes. Finding a way to withdraw this amount of liquid without carrying catalyst with it could be difficult (a large screen area would be required), so a better approach might be to use flash vaporization for cooling:

$$\text{From the simulation, the heat of vaporization} = 377 \text{ kJ/kg}$$

$$\text{Evaporation needed} = 14.94 \times 10^6/(377 \times 10^3) = 39.6 \text{ kg/s}$$

This probably actually increases the required circulation rate, as it would likely be difficult to evaporate much more than about half of the liquid in a flash cooler.

So we must design the reactor circuit to include a heat exchanger that can handle a slurry flow of catalyst. A flow diagram for the proposed reactor design is given in Fig. 15.48. A condenser is used to recover liquid product from the net gas. Some space should also be left at the top of the reactor to allow for vapor–liquid disengagement and for the void space occupied by bubbles, say, an additional 3.66 m, giving an overall tangent length of 6.42 m or 21 ft. The reactor and separation drum can then be designed and costed as pressure vessels; see Chapter 14 and Example 15.4. The heat exchanger and the condenser can be designed using the methods given in Chapter 19. The overall cost will most likely be dominated by the heat exchanger cost.

This design has a number of potential flaws that require further evaluation. The hydraulic performance and mass transfer rate have not been validated, and it would be prudent to construct a pilot plant–scale reactor to confirm the performance. The gas hold-up and bubble volume fraction should be estimated more accurately or determined experimentally in a pilot plant

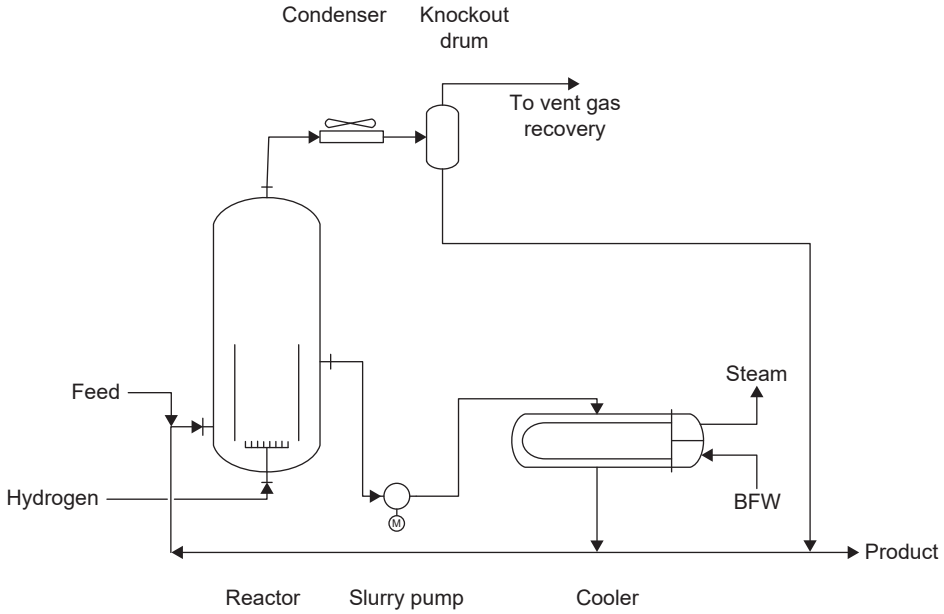


FIG. 15.48 Slurry reactor design for Example 15.5.

reactor to ensure that we have left sufficient space for expansion of the liquid due to bubbles. The use of a cross-flow exchanger will probably give a low F-factor and high area requirement; a different exchanger arrangement might be better. There is also the possibility that catalyst could accumulate in dead spots in the exchanger shell, so flowing the slurry on the tube side might be better.

Several alternative designs could be contemplated. For example, the reaction could be carried out inside a heat exchanger with a suitable design that allowed for gas injection, a loop reactor could be used with the heat exchange tubes in one side of the loop, or the reaction could be combined with product fractionation as a reactive distillation process.

15.9 Design of bioreactors

Biological processing is of increasing importance in the chemical, food, and pharmaceutical industries. Many valuable chemicals and active pharmaceutical ingredients have complex molecular structures that can only be synthesized by biological routes. Some molecules can be made synthetically, but the biological route gives greater selectivity for the desired product or enantiomer. Biological processing can also allow simple chemicals to be produced from biomass feedstocks, as in the fermentation of sugars to ethanol for use as a gasoline additive. Examples of biological processes can be found in almost every sector of the chemical industry; see the design project problems in Appendix E (available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793) for multiple examples.

Biological processing introduces additional constraints on process and reactor design. This section addresses the major concerns that face the design engineer in selecting and sizing a biological reactor and specifying the ancillary equipment required for feed preparation and aseptic operation. There is not sufficient space here to cover the fundamentals of biological processes or the kinetics of biological reactions. These subjects are addressed in biochemical engineering textbooks; see Bailey and Ollis (1986), Blanch and Clark (1996), Shuler et al. (2017), and Krahe (2005).

15.9.1 Enzyme catalysis

If an enzyme can be isolated or expressed from host cells and maintains its activity, it can be used as a catalyst. Enzymes are proteins, usually with between 100 and 2000 amino acid residues, and the active catalytic site is formed by folding of the protein. Enzyme catalysts can be homogeneous in the liquid phase or can be made heterogeneous by immobilization onto a solid support.

Enzyme reactions usually have low reaction rates compared with catalytic reactions of simple molecules at high temperatures, but enzymes can be very selective, particularly when stereoselectivity is required for enantiomeric products.

Enzymes can be permanently deactivated (*denatured*) by high temperatures and can be inhibited by molecules that are able to bind to or block the active site of the enzyme. Enzymes can also lose their activity if the shape of the enzyme molecule is altered, for example, by changes in pH, solution ionic strength or as a result of immobilization. Most enzymes are used in water and lose their activity in organic solvents.

The feedstock for an enzyme reaction is known as a substrate. Substrates can be dissolved in the liquid or can be suspended solids such as starch and fibers in biomass processing. High concentrations of substrate often inhibit the reaction, leading to the selection of a well-mixed reactor or fed-batch reactor. Likewise, enzymes are often inhibited by high concentrations of product.

Some enzymes require the presence of a *cofactor* or *coenzyme* to maintain their function. Cofactors can be as simple as metal ions, ammonia, oxygen, small organic compounds, or vitamins. Cells naturally regulate the levels of cofactors to maintain optimal enzyme performance. In the design of enzyme-catalyzed bioreactors, some experimentation is needed to determine whether make-up of cofactors is needed, as some cofactors are strongly bound, whereas others can be eluted and must be continuously fed.

The kinetics of enzyme-catalyzed reactions are described in all the biochemical engineering books cited in the introduction to this section, as well as in all the reaction engineering books cited in the bibliography at the end of this chapter. Rate equations usually have the form of the Michaelis–Menten equation, which is similar to the Langmuir–Hinshelwood–Hougen–Watson (LHHW) equation for gas–solid catalysis. As is often the case,

biochemical engineering led the way: the Michaelis–Menten equation was developed in 1913, whereas the LHHW equation did not follow until 1947.

The design of a reactor for enzyme catalysis is substantially easier than design for cell cultivation. One of the advantages of enzyme catalysis relative to cell culture is that enzymes do not respire. Consequently, a gas–liquid reactor is not needed unless a gas-phase cofactor is required, which is unusual. Enzyme-catalyzed reactions are therefore usually carried out in the liquid phase or slurry phase if the substrate is a solid. The choice of reactor depends largely on the method of enzyme confinement, as discussed next.

Enzyme confinement and immobilization

Enzymes that can be produced inexpensively can be used once through in a bioreactor; examples include amylase for starch digestion in bread manufacture and the production of high-fructose corn syrup; glucose isomerase for converting glucose to fructose in the manufacture of high-fructose corn syrup and ligninases in paper-making. Enzymes that act on solid substrates must usually be used once through unless the enzyme converts the substrate into soluble components Enzymes that are more expensive must be recovered for recycle or confined to the reactor system.

Most enzymes have large enough molecular size that they can be retained during nanofiltration or ultrafiltration using a membrane filter. If the product molecule is small enough to pass through the filter while the enzyme is retained, the reactor effluent can be sent to a cross-flow filter and the retentate returned to the reactor (Fig. 15.49). This allows the enzyme to be used in solution and confined within the reactor-membrane circuit. The design of membrane filtration processes is discussed in Section 16.5.4.

Many methods have been developed for immobilizing enzymes. The most common approaches are adsorption onto activated carbon, ion exchange resin, functionalized beads or fibers, or encapsulation in a gel. Care must be taken to ensure that the immobilization method does not alter the protein structure of the enzyme and affect its activity. Methods for enzyme immobilization are reviewed by Storey and Schafhauser-Smith (1994). Immobilized enzymes on solid supports can be used in packed-bed reactors if the substrate is dissolved in the liquid phase. A packed bed with recycle is used to achieve a well-mixed performance if the substrate inhibits the reaction (see Fig. 15.33).

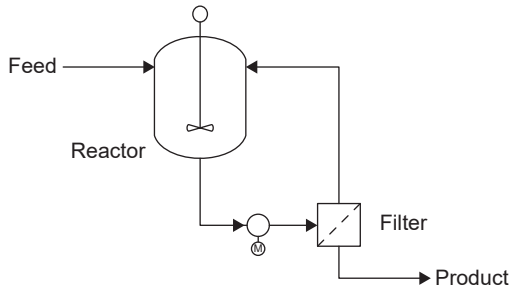


FIG. 15.49 Reactor-membrane circuit for enzyme catalysis.

15.9.2 Cell cultivation

Many biological products are formed through complex reaction paths that are not easily accomplished outside of living cells. In some cases, a species can be found (or bred or otherwise genetically modified) that expresses the desired product into solution. Examples include algae and cyanobacteria that express lipids and yeasts (such as *Saccharomyces cerevisiae*) that express ethanol. For more complex molecules, for example, monoclonal antibodies, it is necessary to break the cell wall (a process known as *lysis*) to harvest the product from inside the cell. The method of product recovery has a large impact on reactor design and even strain selection. For example, if a product is recovered after lysis, the cells should be able to tolerate the product at high concentrations, and a batch or plug flow system is preferred to maximize cell productivity. Conversely, if the cells express product continuously, a fed-batch or continuous well-mixed reactor will often have higher productivity.

Cell cultivation and growth cycle

A wide range of microorganisms can be grown in bioreactors. Most biological processes use simple microorganisms such as bacteria, molds, and yeast. Bacteria and yeast are single-celled organisms, with sizes typically in the range of 0.5 to 2 μm for bacteria and 5 to 10 μm for yeast. Molds are multicellular and have sizes from 5 μm to much larger. Animal and plant cells can also be grown in bioreactors, but the formation of multicellular structures (tissue culture) is much more difficult and is discussed later.

In all cases, the productivity of a bioreactor depends on the concentration of cells in the reactor. The cell concentration will vary with time in a batch or plug flow process and will reach a steady state in a fully continuous process. The reactor concentration of an *intracellular* product (a product inside the cells) will not necessarily be maximized when the concentration of cells is maximized, as long as the product remains stable after cell death. This is illustrated in Fig. 15.50, which illustrates the concentration of live cells and intracellular product during batch fermentation. The fermentation proceeds through the following steps, labeled in the figure:

I. After initial inoculation with cells, there is a short lag phase while the cells adapt to the new environment. During this phase, some of the cells in the inoculum die and balance the rate of cell growth so that overall cell concentration increases only slowly.

II. Once the cells have adjusted to the new environment, their numbers begin to increase rapidly. Because the rate of cell formation is proportional to the number of cells, this is termed the exponential growth phase.

III. Eventually the rate of growth begins to slow, either as a result of nutrient depletion, accumulation of toxic products or by-products, difficulty of obtaining oxygen, or overheating. With careful control of these parameters in a fed-batch or continuous system, a linear growth phase can be maintained for some time. This is important in continuous fermentation for intracellular products, as a fraction of the cells must be harvested continuously to obtain the product.

IV. At some point the rates of cell growth and cell death are in balance and a stationary phase is reached. The goal of continuous fermentation for *extracellular* products (products that are expressed outside the cell) is to sustain this condition by control of nutrient addition, product removal, oxygen supply, pH, and heat removal. In batch fermentation, the stationary phase is often very short.

V. In the final phase, cells die or sporulate and the live cell concentration decreases exponentially. If the desired product is not degraded during or after cell death, then the product concentration in the reactor can continue to increase, even as the live cell population decreases. It may therefore be optimal to continue batch fermentation beyond the end of the stationary phase.

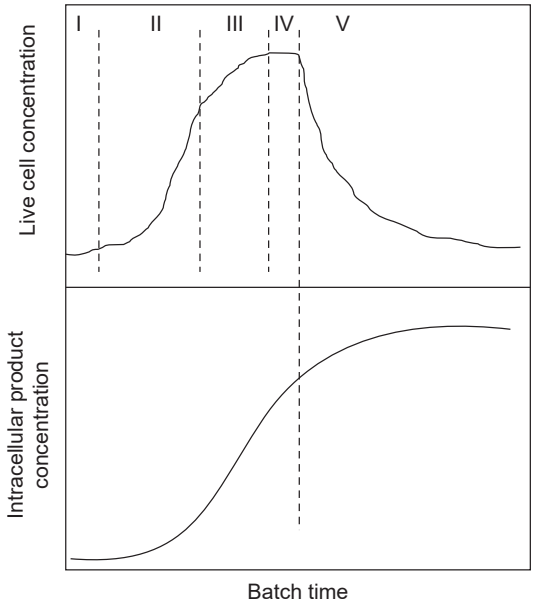


FIG. 15.50 Cell growth and product formation in batch fermentation.

The kinetics of each of these steps can be modeled to develop an overall reaction engineering model of the cell growth cycle and the product formation cycle; see Bailey and Ollis (1986) or Blanch and Clark (1996). In industrial practice, scale-up of fermentation processes is usually accomplished by taking multiple product assays during a small-scale fermentation to determine the optimal cycle experimentally.

Cell immobilization

Cells can be immobilized using many of the same methods used for enzymes, but cell immobilization is less common. Cells already have a large enough size that they are easily retained by filters or even hydrocyclones or centrifuges, and many species naturally flocculate to larger clusters that are even easier to retain. Immobilizing cells onto a support can introduce mass-transfer limitations that reduce cell growth rates and productivity. Consequently, the disadvantages of cell immobilization outweigh the advantages for most processes. The most widely used application of cell immobilization is in biofilters for wastewater treatment, where a film containing many different naturally occurring species forms on a packing and wastewater is passed over the packing. See Bailey and Ollis (1986) for more information on the design of wastewater treatment plants.

Tissue culture

Tissue culture is used to describe the growth of multicellular structures separate from an organism in an artificial environment. The technique has been practiced by biologists on a small laboratory scale for over a hundred years and is used as a method of propagating plants, but is not yet in widespread use as a processing technique. It is, however, of considerable interest to the biomedical industry because of the possibility of growing tissue grafts or even organs for therapeutic uses; see Lavik and Langer (2004) and Xu et al. (2008).

Tissue culture is very difficult to scale up because of the competing needs for high mass transfer and low shear. High mass transfer rates are needed to supply nutrients and oxygen to the cells, whereas low shear rates are necessary to prevent damage to cells and allow multicellular structures to form. Martin and Vermette (2005) and Curtis et al. (2001) review the challenges of tissue culture on a process scale and describe different reactor design approaches, for example, immobilizing the cells on a scaffold or support, such as a fiber bed. This area continues to be the subject of a great deal of research.

15.9.3 Prevention of contamination in biological systems

Biological reactors and their feed systems must be designed to prevent ingress of unwanted species into the reaction medium. The design must consider both chemical and biological contamination, as well as cleaning to prevent batch-to-batch contamination.

Chemical contamination

Cell growth and enzyme activity can be strongly affected by relatively low concentrations of poisons in the growth medium. The reactor and feed system must be designed to ensure that contamination by these chemicals does not occur.

Most biological reactors and feed systems are constructed from low-carbon austenitic stainless steels because of their low rate of corrosion and ease of electropolishing (Krahe, 2005). Although expensive, 316L stainless steel is preferred, but the less expensive 304 and 304L are sometimes used in food processing. Copper and its alloys were used historically in brewing, but have been shown to have a strong inhibitory effect on many fermentation processes, and so copper, bronze, and brasses are usually eliminated from vessels, instruments, valve trims, etc.

Polymers that are used in O-rings, gaskets, valve packing, and diaphragms must withstand the process conditions and be rated as safe for use in food or food packaging if the product is for human or animal consumption. Plasticizers or other additives in the polymer must not leach into solution. Viton, Teflon, and ethylene-propylene-diene rubber (EPDM) are most often used.

Process feed quality must be carefully controlled for the presence of potential contaminants or poisons. Processes that make products for human or animal consumption do not necessarily require USP-grade feeds, but the feed quality or processing must be such that USP-grade product quality is attained.

Additional requirements on feed purity and quality control may be set by Good Manufacturing Practice (GMP) regulations; see Section 15.9.8.

Biological contamination and design for sterile operation

If a different species enters a fermenter, it can compete with the design species for substrate, cause infection and cell loss, or contaminate the products with unwanted and potentially toxic compounds. Biological processes are therefore almost always designed for aseptic operation. The maintenance of aseptic conditions requires careful cleaning between batches or continuous runs, sterilization of the plant before operation, and sterility of every feed other than the inoculum that is introduced during normal operation.

Sterilization is itself a reaction process, and the rate of death of biological contaminants can usually be described with first-order kinetics; however, because biological contaminants must be essentially completely removed, the process is often treated in probabilistic terms.

Production equipment is too large to be disassembled and sterilized in autoclaves, so sterilization in place (SIP) is used for the plant. Sterilization of the plant is carried out in batch mode, typically by using steam to heat the plant to a high enough temperature (usually 120 °C or higher) followed by holding at temperature for a predetermined time and then cooling back to reaction conditions. During cooling, steam in the plant will condense, and air must be admitted to prevent underpressuring, so it is important that the air source also be sterile.

Feed media pose several sterilization challenges. Simple compounds such as sugars and salts can be dissolved in water and sterilized by heating to high temperature, but some nutrients such as vitamins are thermally sensitive and cannot be heat treated without losing some material to degradation; see Leskova et al. (2006). In batch fermentation, those feed components that are not thermally sensitive can be charged to the reactor and sterilized along with the plant. In fed-batch and continuous processes, the feed must be continuously sterilized. Because of the importance of ensuring complete conversion (death of biological contaminants), plug flow devices must be used.

The most common flow schemes for continuous sterilization are shown in Figs. 15.51 and 15.52. Fig. 15.51 shows a steam injection sterilization process, in which steam is injected into the liquid feed to cause heating. The liquid is then passed through a serpentine tubular holding section to achieve the desired residence time for sterilization and cooled to the process temperature by flash cooling. Flash cooling reduces the possibility of contamination from cooling water in a cooler. Fig. 15.52 shows a heat exchange sterilization process using plate heat exchangers. Heat from the product is recovered to pre-heat the feed before it enters a steam heater. The feed is then held at temperature in a tubular holding section before being cooled against incoming feed and cooling water. Plate exchangers are typically used because of their ease of cleaning and inspection. Heat-exchange sterilization has lower energy costs but has a higher possibility of feed-to-product contamination or contamination from cooling water.

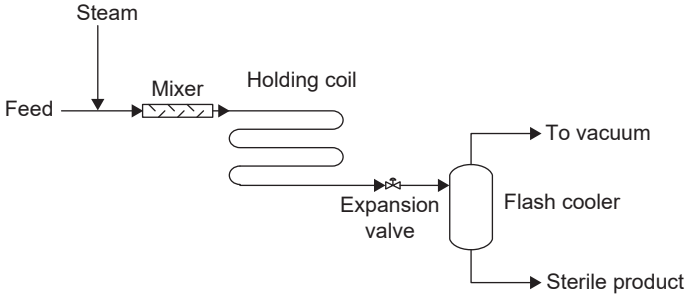


FIG. 15.51 Steam injection sterilization process.

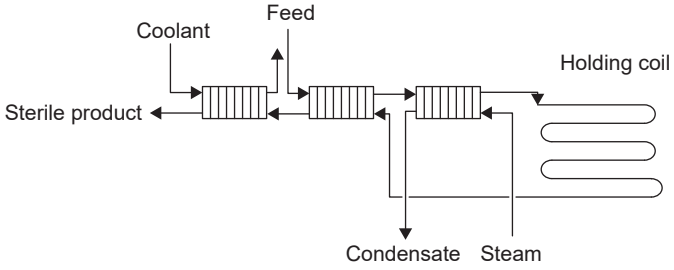


FIG. 15.52 Heat exchange sterilization process.

The holding time required for sterilization depends on the temperature used, the degree of sterility required, and the types of organism that might be present in the feed. Fifteen minutes at 120 °C or three minutes at 135 °C are typical treatments that are adequate for bacteria, molds, fungi, and bacterial spores, but more extreme treatments are used in some cases.

If thermally sensitive compounds such as vitamins are subjected to heat treatment, then high temperatures must be used with short residence times to minimize thermal degradation of the desired component (*high-temperature short-time*, or HTST, sterilization). It may be necessary to prepare a feed that contains a higher concentration of the desired component to allow for some thermal loss during sterilization. Continuous sterilization processes are more suited to HTST conditions than batch sterilization in the reactor, as cooling occurs more quickly in continuous flow. In extreme cases, a sterile feed may need to be purchased or synthesized.

Some components that are introduced into a fermenter may not require sterilization. For example, if acids or bases are used to control pH, their concentration may be high enough to guarantee sterility without sterilization.

Air that is brought in as a source of oxygen is usually sterilized by membrane filtration to remove bacteria and particulates. Air leakage into the plant from the atmosphere is normally prevented by operating the process under pressure. The exception is for species that are strong pathogens, where the hazard posed to workers from a potential leak is too great and the plant is run under slight vacuum.

Cleaning

Cleaning of the plant is required at the end of a production run to remove residual substrates that can lead to contamination and to prevent batch-to-batch contamination. Bioreactors and their feed systems are usually designed for cleaning-in-place (CIP), but disassembly and manual cleaning are used for equipment, such as heat exchangers, that is prone to fouling.

Bioreactor systems should be designed to be free-draining and to avoid corners, crevices, and dead-ended pipe legs to facilitate cleaning. Plate heat exchangers are preferred over shell and tube heat exchangers for ease of cleaning, as they have no internal dead spots where material can accumulate and are easily taken apart and inspected; see Section 19.12. Diaphragm valves are also preferred because of their ease of cleaning.

Cleaning cycles typically consist of the following steps:

1. Wash with high-pressure water jets
2. Drain
3. Wash with alkaline cleaning solution (typically 1M NaOH)
4. Drain
5. Rinse with tap water
6. Drain
7. Wash with acidic cleaning solution (typically 1M phosphoric or nitric acid)
8. Drain
9. Rinse with tap water
10. Drain
11. Rinse with deionized water
12. Drain

The acid and alkaline washes may be reversed, depending on the system.

Cleaning cycles typically require filling and emptying the reactor repeatedly and can contribute significantly to the time between batches in batch fermentation. The process design must include the necessary equipment for preparing the cleaning fluids (typically by dilution of stronger acid or base), as well as neutralizing and disposing of the effluents from cleaning. Equipment cleaning has a substantial impact on wastewater production in biochemical processing, and hence a significant environmental impact. Previs and Roche (2018) discuss methods to reduce the environmental impact of cleaning processes.

15.9.4 Feed preparation and consumption

Even single-celled organisms require a balanced diet to grow happily and reproduce. The feed medium must contain sources of carbon, nitrogen, phosphorus, sulfur, and required metal ions. In some cases, more complex components such as vitamins or enzymes may be added.

TABLE 15.13 Typical feed medium composition

Component	Composition (g)
Water	1000
Glucose	5
NH_4Cl	1
K_2HPO_4	1
$MgSO_4.7H_2O$	0.2
$FeSO_4.7H_2O$	0.01
$CaCl_2$	0.01
Mn, Mo, Cu, Co, Zn (as salts)	2×10^{-5} to 5×10^{-4} of each

From Stanier et al. (1986).

The optimum feed medium depends on the organism (or enzyme), desired product, method of production (extracellular or intracellular), and choice of fermentation reactor (batch or continuous). The recipe is usually determined experimentally. A typical composition, taken from Stanier et al. (1986) is given in Table 15.13.

Cell metabolism and productivity can be manipulated by changes in feed composition. It may be desirable to change the feed during different phases of the growth cycle shown in Fig. 15.50. For example, more minerals may be needed during the exponential growth phase, but a change in composition may prolong the stationary phase or lead to a higher titer of product. Mead and Van Urk (2000) describe a process for controlling medium concentration in response to a by-product concentration, and Shibuya et al. (2010) describe a method for controlling feed composition by mixing several media to optimize overall productivity.

It is important to note that in most biological processes the rate of feed consumption is determined primarily by cell metabolism and growth of new cells and has no strong correlation to the rate of product formation. A stoichiometric relationship between the feed and product (or even feed and cell mass) may have no value for design purposes. Cells require nutrients both to maintain life and to grow new cells. If the rate of growth of new cells, μ_g, is defined by:

$$\frac{\mathrm{d}\,x}{\mathrm{d}\,t} = \mu_g x \tag{15.29}$$

where:

x = concentration of cells, g/l
t = time, s
μ_g = growth rate, s^{-1}

then the rate of consumption of any substrate can be written as:

$$\frac{\mathrm{d}\,s_i}{\mathrm{d}\,t} = \left(m_i + \frac{\mu_g}{Y_i}\right) x \tag{15.30}$$

where:

s_i = concentration of substrate i, g/l
m_i = rate of consumption of substrate i to maintain cell life, g of substrate/g cells.s
Y_i = yield of new cells on substrate i, g of cells/g substrate

Some example values of m and Y for glucose and oxygen for different species are given in Table 15.14, based on data from Solomon and Erickson (1981).

TABLE 15.14 Substrate consumption for cell maintenance and growth

Microorganism	$m_{glucose}$ (g/g.hr)	$Y_{glucose}$ (g/g)	m_{oxygen} (g/g.hr)	Y_{oxygen} (g/g)
Escherichia coli	0.072	0.35	0.6	24.7
Escherichia coli	0.090	0.53	3.0	42
Saccharomyces cerevisiae	0.018	0.51	0.6	34.5
Aerobacter aerogenes	0.054	0.38	1.4	44

From Solomon and Erickson (1981).

Rates of cell growth vary widely by species. Green and Southard (2018) state typical rates of biomass growth are in the range 2 to 5 g/liter.h, and typical rates of oxygen consumption are in the range 1.5 to 4 g/liter.h.

15.9.5 Batch fermentation

Most biological processes are carried out using batch fermentation reactors. Batch operation is easier to scale up from laboratory-scale fermentation, and batch integrity is an important method of quality control.

In strict batch cultivation, the substrate is charged to the reactor, sterilized and cooled, and then the inoculum of live cells is added. No additional substrate is added, although air is usually added continuously to maintain the oxygen concentration above a critical level. The critical oxygen level varies by species, but is typically above 1 ppm. After a set period of time, the fermentation is stopped and the reactor contents sent to downstream processes for harvesting.

Strict batch processing is rather inefficient, as the rate of cell growth and the product titer quickly become limited by consumption of substrate. A more common approach is fed-batch cultivation, in which additional feed medium is added as the cell concentration increases, allowing the process to proceed further into the growth cycle and achieve higher product titers. In a fed-batch process, the reactor may start out only 20% to 40% filled to allow space for adding more growth medium, and the design must ensure that mixing and aeration will be sufficient at all fill levels. Different fed-batch processing strategies are described in Krahe (2005).

Fermenter design

Batch fermenters are usually stirred tanks with jackets and/or coils for heating and cooling and spargers or other means for introducing air. A typical design is shown in Fig. 15.53.

Good mixing is important in fermentation to ensure that all the microorganisms in the fermenter have access to the desired concentrations of substrates and oxygen and to maintain isothermal conditions. Baffles are usually used to improve the mixing pattern in the vessel and prevent swirl (see Section 15.5.2), but baffles can make cleaning and sterilization more difficult. Other mixing criteria for stirred tanks are discussed in Section 15.5.2.

The rate of agitation in a fermenter is usually determined primarily by the rate of oxygen mass transfer that is needed, and the agitation rate can be adjusted to give the desired mass transfer parameter, $k_L a$; see Equations 15.13 to 15.15 in Section 15.3.4. The cells have a density that is very close to the density of water, so they are easily suspended in solution, and biomass suspension rarely limits the agitation rate. Very high agitation rates are avoided, as high shear can cause breakage of the cell walls, causing death.

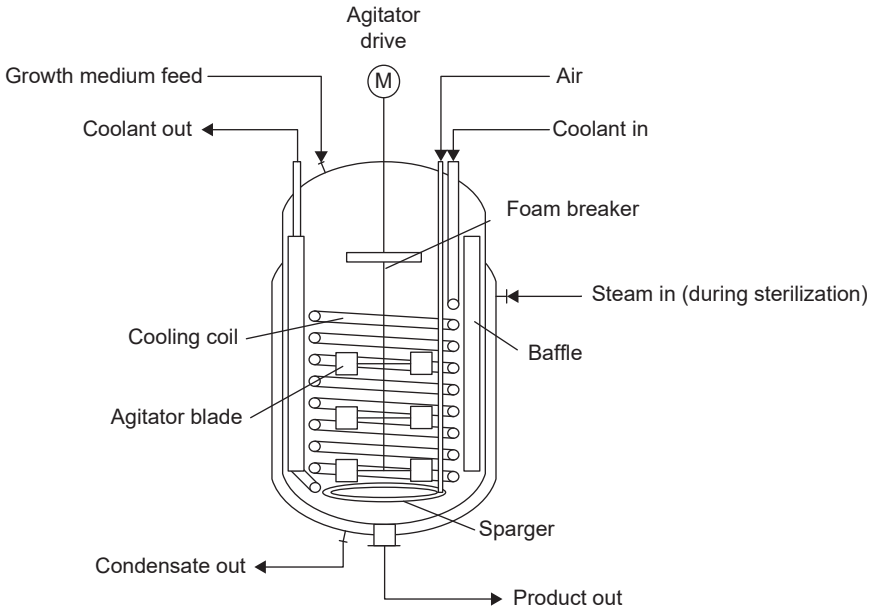


FIG. 15.53 Fermentation reactor.

TABLE 15.15 Standard fermenter sizes

Vessel size (m^3)	0.5	1.0	1.5	3	5	7.5	15	25	30
Vessel size (gal)	150	300	400	800	1500	2000	4000	7000	8000

Foaming can be a serious problem in fermentation. Surfactants may be present in the growth media or formed during fermentation. The bubbling of air naturally causes froth to form at the vapor–liquid interface. If foaming is excessive, cells and product can be lost to the vapor recovery system and reactor productivity impaired. Mechanical foam breakers mounted on the agitator shaft can be used to break up large bubbles. Antifoaming agents (antifoam) can be added if a suitable compound can be identified that does not interfere with the cells or impede oxygen transfer. The reactor is usually designed to operate less than 75% filled to allow space for foam breaking and vapor–liquid segregation.

The rate of heat release in fermentation processes is usually relatively low, and adequate cooling can be provided by an external jacket or internal coils for smaller fermenters. As was the case for baffles, the presence of coils can make cleaning and sterilization more difficult. The rate of heat transfer can be found using the correlations given in Section 19.18.

The size of a batch fermenter is determined by the species productivity, required residence time and desired plant attainment rate. Larger-size fermenters are custom-built, but standard vessel sizes are used at small and intermediate scales. Standard sizes are usually stated in liters or m^3, and the more common sizes are given in Table 15.15, with approximate equivalents in U.S. gallons. The vessel aspect ratio is usually between 2 and 4. Krahe (2005) and Benz (2019) discuss factors to consider in choosing between a taller or shorter vessel.

When the batch residence time is long, it is common to use several reactors in parallel so as to maximize the productivity of downstream separation equipment. Very large fermenters are only used for inexpensive products so that contamination of a batch does not cause excessive financial loss. For example, Lee (2010) stated that a typical new plant for monoclonal antibody production would have 4 to 12 fermenters, each of 10 to 25 m^3. After 10 to 14 days of culture time, each fermenter would attain a titer of about 4 g/l of product. The total plant cost, including feed preparation and product recovery, would be between $400 million and $1 billion, and the plant would take about 6 years to build from groundbreaking to Food and Drug Administration (FDA) approval.

Most production-scale batch fermenters are made from austenitic stainless steel, typically 316L, to avoid contamination of the growth medium with corrosion products. Stainless steel fermenters are designed as pressure vessels so as to withstand sterilization conditions; see Chapter 14. At smaller production volumes, there is a growing market for single-use disposable plastic reactors, which now account for about 75% of clinical-scale production of FDA GMP–certified materials and about 5% of commercial-scale production (Mullin, 2016). Disposable reactors are available in sizes up to 2 m^3 at the time of writing. Thayer (2010) gives details of suppliers and applications of disposable vessels.

Smaller batch fermenters are often emptied by pressuring the vessel with air to force the liquid out through the bottom drain line. This obviates using a bottoms pump and removes a potential source of contamination at the pump shaft seal.

Scale-up considerations

Batch fermentation is used industrially at very large scales. Beer and wine brewing can be carried out using either continuous or batch fermentation, with fermenter volumes up to 200 m^3 quite common. Even very expensive products such as monoclonal antibodies are routinely produced in 25-m^3 batches (Lee, 2010).

Scale-up of batch fermenters is simple in the sense that small-scale fermentations are also batch processes, so scaling of kinetics data is relatively straightforward as long as the same temperature and concentrations of substrates and oxygen can be achieved in the larger vessel. Scale-up is not trivial, however, as rates of heat and mass transfer become increasingly important as fermenter size is increased.

The most important factor in scale-up of a batch fermentation process is usually ensuring that the same oxygen concentration can be maintained. The designer should attempt to ensure that the new design will obtain the same mass transfer parameter, k_La, which may require increasing the agitation rate or air flow rate compared with a smaller vessel. The rate at which air can be supplied is often the limit on the maximum concentration of live organisms that can be attained.

The rate of heat transfer can also be an important consideration in scaling up a batch fermentation process. Most fermentation processes are mildly exothermic. If heat is not removed, the temperature will slowly increase until cell

productivity decreases or cells begin to die. A larger fermenter has a lower external area per unit volume, and so the rate of heat loss to the environment is lower in proportion to the rate of heat generation. Additional cooling means, such as cooling coils or an external pumped heat exchange circuit, may need to be considered.

The scale-up of batch fermentation processes is discussed in the context of pharmaceuticals manufacture in the book by Levin (2011).

15.9.6 Continuous fermentation

In continuous fermentation, the plant is operated such that the rate of live cell loss (either by death or elutriation from the fermenter) matches the growth rate of new cells. A stable population balance is thereby achieved, and with careful control, this steady state can be maintained for days, weeks, or even months. Steady continuous operation maximizes the volumetric productivity of the fermenter, as the fraction of time spent in draining, cleaning, filling, and sterilizing operations is dramatically reduced.

The design of a continuous fermentation reactor is strongly dependent on whether the product is extracellular or intracellular.

Extracellular products can be recovered from the fermentation broth without requiring removal of the cells. The cells can therefore be contained in the reactor loop, either by immobilization or by using a reactor-membrane circuit, as shown in Fig. 15.49. Reactor productivity will usually be optimized if the cells are in the stationary phase of the growth cycle, shown as phase IV in Fig. 15.50, with the highest stable concentration of live cells. The rates of substrate addition, dilution (by water coming in with the substrate), oxygen addition, carbon dioxide removal, and heat removal must all be controlled to maintain the optimal conditions for sustaining this steady state. The most common industrial example of continuous fermentation for an extracellular product is the use of *S. cerevisiae* to ferment sugars into alcohol in production of ethanol for use in gasoline and in large-scale brewing of wine and beer.

When the product is the cells themselves or the product must be harvested from inside the cell by lysis, a continuous fermentation process must maximize the production of live cells. Cells are usually removed by elutriation, either from the reactor itself or by using a settling vessel, ultrafiltration module, or hydrocyclone to form a product stream that has a higher cell concentration than the fermentation broth. The reactor is usually a continuous stirred tank fermenter (CSTF), often referred to as a *chemostat*. Reactor productivity is maximized by operating at a point on the growth cycle with a high cell growth rate, typically in the linear phase of the growth cycle, shown as phase III in Fig. 15.50, and reactor conditions are chosen to stimulate cell growth. Most nutrients are supplied in excess so that one nutrient becomes the limiting feed and can be controlled to control the growth rate. Continuous fermenters with cell harvest are used in the production of bakers' yeast and in the manufacture of certain bulk enzymes.

Continuous fermenter design and scale-up

All of the issues discussed under batch fermentation in Section 15.9.5 also apply to CSTFs, with the additional requirement that the reactor must be designed for cell retention or elutriation, depending on the method of product recovery. Continuous stirred tank fermenters have the same appearance as batch fermenters (see Fig. 15.53).

The maximum concentration of cells that can be achieved in the fermentation broth is typically only a few weight percent, so it is advantageous to concentrate the cells into a thicker slurry product when the product is intracellular or is the cells themselves. Concentrating the cells reduces the volume flow of water through the plant, reduces the size of product recovery operations, allows use of more concentrated feeds, and reduces the sterilization requirements. If the cells are not too sensitive to shear, hydrocyclones can be used. Alternatively, ultrafiltration can be used to reject water, or a settling tank can be used. The design of equipment for separating solids from liquids is discussed in Section 18.6.

Sterility of all feeds to the process is critical to the operation of a continuous fermenter; see Section 15.9.3. Sterile conditions must also be maintained in immediate downstream operations, as bacteria are able to travel upstream against the product flow. Product quality must be monitored regularly to ensure that contamination has not occurred. Continuous processes cannot use batch integrity as a means of quality control. If contamination occurs, the run must be stopped and the vessel emptied, cleaned, and sterilized before being placed back in service.

As with batch fermentation processes, the primary concerns in scale-up are ensuring adequate rates of mass transfer for oxygen and carbon dioxide and ensuring adequate heat removal for good control of temperature. Heat removal is somewhat easier in a continuous fermentation than in batch fermentation, as the continuous flow of feed and removal of product allows use of a cold feed, and hence reduces the cooling requirement.

Reactors for immobilized cells can have a variety of geometries. Immobilized cells still require oxygen for respiration, so slurry reactors, trickle beds, or fluidized reactors must be used. The design of these reactors is similar to reactors for solid-catalyzed vapor–liquid reactions and is discussed in Section 15.7.5. Immobilization of cells that can be grown in suspension is rarely practiced industrially, as it is much harder to provide good heat and mass transfer to immobilized cells. Cell immobilization is discussed in more detail in Section 15.9.2.

15.9.7 Bioreactor instrumentation and control

The conditions that must be controlled in a bioreactor typically include the following:

- **Temperature:** is usually measured by one or more thermocouples and controlled by manipulating the rate of flow of steam or coolant to the jacket, coils, or external heat exchanger.
- **Pressure:** is usually measured on the vent gas line and controlled by a vent gas pressure control valve. Pressure is usually maintained above ambient to prevent contamination from air leaks into the plant.
- **Liquid level:** is important in control of fed-batch and continuous fermenters. Liquid level can be difficult to measure due to gas bubbles and foam in the reactor. Load cells are sometimes used to infer the total vessel contents for smaller reactors. Alternatively, the pressure difference between the top and bottom of the reactor can be measured and hence the liquid volume inferred from the static head. This method determines the liquid content but does not locate the vapor–liquid interface.
- **Feed rate:** in fed-batch and continuous fermentation processes, the rate of substrate addition must be maintained in the desired range. Feed rate is often varied during a batch or during a continuous production cycle, and the rates of individual feed components may also be varied to maximize productivity. It is common to use a more dilute growth medium at the start of the fermentation and then add more concentrated feeds later in the run to limit dilution and cell washout.
- **Agitation rate:** stirrer speed is usually continuously controlled to maintain the desired level of agitation.
- **pH:** *in situ* pH sensors are used to measure pH. The pH is controlled by discrete (on/off) addition of small amounts of a concentrated acid or base such as sulfuric acid, sodium hydroxide, or ammonia solution.
- **Dissolved oxygen:** the oxygen concentration is usually measured by an *in situ* oxygen probe. The oxygen detector can control the rate of air addition or can be cascaded onto the pressure controller (to increase oxygen partial pressure by increasing overall pressure) or the agitation rate controller (to increase mass transfer by higher agitation).
- **Foaming:** many fermenters are fitted with a foam detector to control the rate of antifoam addition. This is a simple conductivity probe placed at a suitable height above the liquid level and shielded from splashing.

Gas outlet composition is sometimes monitored as a means of measuring the oxygen availability or carbon dioxide production rate. Liquid concentration is usually determined using off-line chromatography methods. Methods for measuring cell concentrations are described in Bailey and Ollis (1986).

Batch fermenters use programmable logic controllers to control the sequence of events during a batch run and to ensure that all steps are carried out in the correct order. Programmable logic controllers are also used for discrete (on/off) control of some operations in CSTFs and for control of cleaning and sterilization operations.

More information on the control of biological reactors is given by Alford (2009).

15.9.8 Safety and quality control of bioreactors

Biological processes are typically carried out in aqueous solution under conditions that sustain life, and consequently are substantially less hazardous than nonbiological processes that handle flammable mixtures at high temperatures and pressures. Nonetheless, microbes and biologically active products can be a hazard to workers and the environment and must be contained in the plant. In addition to complying with safety regulations, plants that make products that are intended for human or animal consumption are required by law to maintain rigorous quality control standards and must undergo periodic inspection by regulatory agencies.

Batch processing is an important quality control method in biological processing. The use of batch processing allows operators to maintain batch integrity throughout processing, that is, to keep the same batch of material together and not mix it with other batches as it moves through the different stages of the process. The plant is cleaned and sterilized between batches so that batch-to-batch contamination cannot occur. If a batch is found to be contaminated or fails to meet quality control requirements, the entire batch can be rejected and sent to waste disposal without affecting any other batch, because no batch should ever come into contact with any other batch.

Good Manufacturing Practices

The widespread use of biological processing in the manufacture of food additives, personal care products, cosmetics, and drugs brings many products under the jurisdiction of the FDA in the United States, and therefore subject to production using CGMP (GMP for short). Other countries have their own GMP requirements, but all of them are similar to those of the World Health Organization (WHO) for pharmaceuticals manufacture. The WHO guidelines are set out in WHO Technical Report Series 908, which is available for free download from www.who.int/medicines/areas/. Information on U.S. GMP requirements is given in 21 CFR Part 210 and 21 CFR Part 211 and can be obtained from the FDA at www.fda.gov; see also Willig and Stoker (1996), Nally (2006), and Bunn (2019).

Food ingredients and drugs manufactured in the United Stated must be made to the standards specified by the United States Pharmacopeia (USP). Food ingredients are covered in the USP Food Chemicals Codex (FCC) set of standards. USP and FCC standards are recognized internationally and have been adopted as legal standards in many other countries.

Similar requirements are in force in Canada, and details of Canadian GMP guidelines can be obtained from Health Canada at www.hc-sc.gc.ca.

The GMP guidelines spell out the requirements for quality assurance, including maintenance of a quality control system, plant and facility design and operation, sanitation and hygiene, training, record keeping, inspection, subcontractor management, and materials testing.

Containment

Containment of biological material inside the plant is important in the following situations:

- When the microorganisms in the plant are pathogenic to humans, wildlife, or plants.
- When the microorganisms produce compounds that are toxic through their metabolism.
- When exposure of workers to the microorganism can lead to allergic reactions.
- When the microorganisms have been genetically modified to have desirable properties and there is a concern that the organism could interbreed with wild species if released into the environment.

For example, at the time of writing there is a great deal of research interest in genetically modified algae that have rapid growth rates and use sunlight to convert carbon dioxide into oils with high efficiency. These species might be very attractive as a means of mitigating carbon dioxide emissions, but could be difficult to control if they were to escape into the environment and hybridize with natural algae.

The primary means of containment of the liquid phase is the plant itself. Open-air transfers are avoided for sterility and quality-control reasons. Leakage through valve-stem or pump-shaft seals is also usually prevented by the selection of leakproof equipment as a means of preventing contamination from entering the plant.

Containment of biological hazards in the reactor off-gas is more difficult. The agitated, bubbling conditions in the fermenter are likely to lead to some entrainment of spray in the off-gas. If the spray contains microorganisms or their spores, then it must be treated to prevent leakage to the environment. High-efficiency particulate air (HEPA) filters are usually used on the off-gas, with multiple stages for more hazardous organisms. In extreme cases, incineration of the off-gas may be required. Krahe (2005) provides a guide to the selection of off-gas treatment technology.

Example 15.6

Riboflavin (vitamin B_2) is a nutrient that is used as a food additive (mainly in animal feed, but also in breakfast cereal). It can be produced by fermentation of glucose using strains of the yeast species *Candida famata*, as described in US 5,164,303 (Heefner et al., 1992). Example IV in the patent gives the following yields in a 450-liter fed-batch fermentation tank operated at 30 °C and 40% of oxygen saturation. The glucose concentration was maintained above a critical level of 30 g/l by feeding additional 600 g/l glucose solution during the fermentation.

Time	Optical density	Riboflavin	Glucose
(h)	(620 nm)	(g/l)	(g/l)
0	0.06	0.0	68.8
40	25.0	0.0	47.8
60	50.0	2.5	32.2
80	150	6.0	43.0
100	175	9.0	47.9
140	225	15.0	44.5
200	210	21.0	47.2

Design a reactor system to produce 40 metric tons per year of riboflavin using the strain given in the patent.

Solution

Estimate reactor volume

A quick calculation of the overall productivity will give an initial estimate of the required reactor volume.

$$\text{Riboflavin production} = 21 \text{ g/l in } 200 \text{ h} = 21/200 = 0.105 \text{ g/l.h or } 0.105 \text{ kg/m}^3\text{.h}$$

$$\text{Assuming 8000 operating hours per year, productivity} = 8000 \times 0.105 = 840 \text{ kg/m}^3\text{.y}$$

$$\text{So to produce 40 t/y, at 100\% fermenter utilization would require } 40/0.84 = 47.6 \text{ m}^3$$

We do not expect that batch fermentation could run at 100% utilization, as we need to allow time for CIP and SIP between batches. If we make an initial assumption that CIP and SIP account for half the total time, then the utilization would be 50% and the required volume $47.6 \times 2 = 95.2$ m^3. Assuming that the reactors are 75% full at the end of a batch, the total volume needed is $95.2/0.75 = 127$ m^3. If we add another reactor to allow for one to be under extended maintenance at any time, then six 25-m^3 standard fermentation reactors looks like a good initial design.

Determine cleaning time

We now need to determine the cleaning and heat transfer requirements to confirm that the design basis CIP and SIP times can be accomplished.

$$\text{Liquid content of 75\% full 25-m}^3\text{ fermenter} = 0.75 \times 25 = 18.75 \text{ m}^3$$

$$\text{Time to drain vessel through a 6-inch pipe at 1 m/s} = \frac{18.75}{1 \times \pi \times (6 \times 0.0254)^2/4} = 1028 \text{ s}$$

This is about 17 minutes, which is not unreasonable. Using an 8-inch pipe would give a drain time of 9.6 minutes, which might be preferred, but there are probably fewer pipe fittings and valves suitable for sterile service at the larger size, so let us select 6-inch for now and assume a drain time of 20 minutes to allow some time for pressuring the vessel during draining.

The washing step depends on the number of nozzles and the flow through each nozzle. BETE Fog Nozzle, Inc., is a nozzle manufacturer that sells a wide range of nozzles for cleaning applications. Their SC24 deluge washing nozzle can deliver 272.5 l/min at 4.5 bar. If we assume that we will fill the vessel to 80% full during cleaning (20 m^3), then at this flow rate, using six nozzles, the time required to fill the reactor to 20 m^3 would be $20 \times 10^3/(6 \times 272.5) = 12.2$ minutes. The time to drain from 80% full is $1028 \times 80/75 = 1097$ s, or about 18.3 minutes, so still under the allowed 20 minutes.

Following the guidance in Section 15.9.3, we can now propose the following CIP cycle:

1. Wash with high-pressure water jets (12 min spray + 8 min agitation)
2. Drain (20 min)
3. Wash with 1M NaOH (12 min spray + 8 min agitation)
4. Drain (20 min)
5. Rinse with tap water (12 min spray + 8 min agitation)
6. Drain (20 min)
7. Wash with 1M phosphoric acid (12 min spray + 8 min agitation)
8. Drain (20 min)
9. Rinse with tap water (12 min spray + 8 min agitation)
10. Drain (20 min)
11. Rinse with deionized water (12 min spray + 8 min agitation)
12. Drain (20 min)

$$\text{Total CIP time} = 12 \times 20 = 240 \text{ minutes} = 4 \text{ hours}$$

Determine SIP time

The sterilization and cool-down is a little more difficult to evaluate. The reactor is only partially filled at the start of the run, as this is a fed-batch process. It is clear from the glucose concentration data that additional glucose is being fed after 60 hours, so we need to make a rough estimate of the initial volume in the reactor. This information is not available in the patent, so some creative interpretation is required.

Fig. 15.54 shows the optical density (a measure of total cell mass, including live and dead cells) and riboflavin concentration plotted against time. Note that the figure is similar to Fig. 15.50, with the maximum product concentration attained after the peak in cell mass. It is impossible to tell from this figure where the maximum optical density was obtained, but it looks like

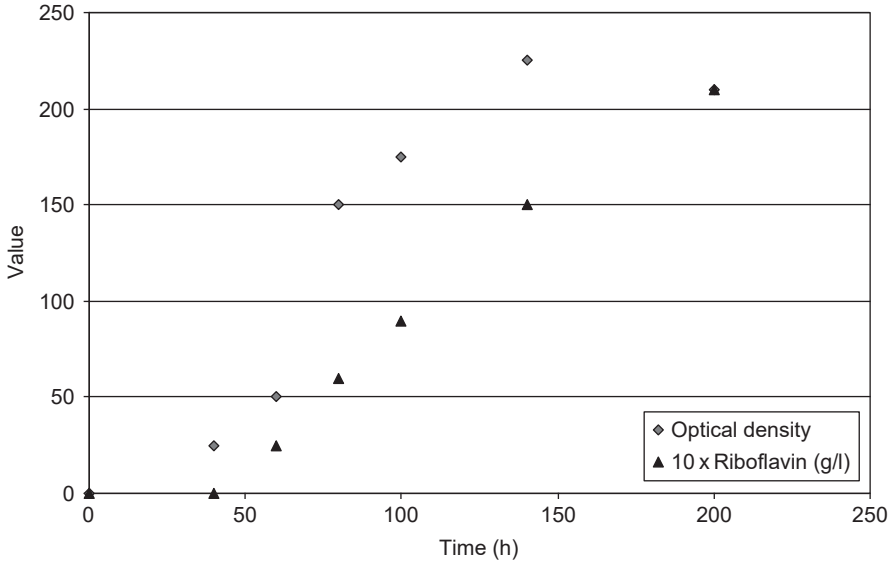


FIG. 15.54 Cell and product yields for Example 15.6.

it was some time between 140 and 200 hours. Because this is a batch process, the only way that the cell mass can decrease is by dilution. We can hence calculate how much liquid was added in the last 60 hours:

$$\text{If the cell mass is } x, \text{ then the density at the end of the run is : } 210 = \frac{x}{18.75}$$

$$\text{If the liquid volume added is } y, \text{ then the density at 140 hours is } 225 = \frac{x}{18.75 - y}$$

$$\text{Hence: } \frac{18.75 - y}{18.75} = \frac{210}{225}\ , \ y = 1.25\ \text{m}^3$$

The rate of dilution with fresh growth medium is highest at the end of the run when the concentration of cells is highest. Earlier in the run, beginning some time around 60 minutes, the required rate of glucose addition would be lower. The total time over which material is fed to the reactor is $200 - 60 = 140$ minutes, and 1.25 m^3 is added in the last 60 minutes, so a reasonable assumption of the total volume added is somewhere between 2 and 2.5 m^3. For the purposes of designing the sterilization, we should take a conservative estimate and use 2 m^3, as this gives the largest estimate for the initial volume in the reactor. The initial volume in the fermenter is then $18.75 - 2 = 16.75$ m^3 of growth medium. The growth medium is largely water, and we can assume the properties of water for the heat transfer calculations.

To determine the heating and cooling times, we need to make an unsteady-state heat balance on the fermenter. If the vessel is heated using a steam jacket, with constant wall temperature, the rate of change in temperature of the contents is equal to the rate of heat transfer across the wall:

$$m_L C_p \frac{\mathrm{d}\,T}{\mathrm{d}\,t} = U\,A\,(T_w - T) \tag{15.31}$$

$$\text{Hence : } T = T_w - (T_w - T_o)\exp\left\{-\left(\frac{U\,A}{m_L\,C_p}\right)t\right\} \tag{15.32}$$

where:

m_L = mass of liquid in the fermenter = 16.75×10^3 kg
C_p = specific heat capacity of contents = 4.2 kJ/kg°C
U = the overall heat transfer coefficient, kW/m^2°C
A = heat transfer area, m^2
T = temperature, °C
T_w = wall temperature, °C
T_o = initial temperature, °C
t = time, s

The jacket area can be estimated from the reactor dimensions. A 25-m^3 vessel with 2:1 aspect ratio has diameter $(25 \times 2/\pi)^{1/3} = 2.515$ m. If this vessel is filled with 16.75 m^3 of liquid, then it is filled to a depth of $2.515 \times 2 \times 16.75/25 = 3.37$ m, and the available area for heat transfer is $\pi \times 2.515 \times 3.37 = 26.6$ m^2.

The overall heat transfer coefficient can be estimated from Table 19.1 to be about 700 W/m^2K. To confirm this value, we can use Equation 19.70c:

$$\mathrm{Nu} = 0.74\,\mathrm{Re}^{0.67}\,\mathrm{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.70c}$$

where μ_w is the viscosity at the wall. The Prandtl number for water over the temperature range of interest (20 °C to 120 °C) varies from 7 to about 1.4, so as a conservative estimate use 1.5.

The Reynolds number for an agitated vessel was given in Equation 15.16 as:

$$\mathrm{Re} = \frac{d_a^2 N \rho}{\mu}$$

Where:

ρ = fluid density $\approx$ 1000 kg/m^3
μ = fluid viscosity $\approx 0.4 \times 10^{-3}$ Ns/m^2 over the temperature range of interest
N = agitator speed, s^{-1} (revolutions per second) (rps)
d_a = agitator diameter = 0.6 × vessel diameter = 1.51 m

The power number, N_p, was also given in Equation 15.16:

$$\mathrm{N_p} = \text{power number} = \frac{P_a}{d_a^5 N^3 \rho}$$

Where:

P_a is the power consumption in W.

From Table 15.5, for mild agitation we need a power input of ~0.05 kW/m^3, so:

$$P_a = 0.05 \times 1000 \times 16.75 = 837.5 \text{ W}$$

From Fig. 15.16, the power number is about 4 at high values of Re (using curve 1), so:

$$\mathrm{N_p} = 4 \times \frac{837.5}{1.51^5 \times N^3 \times 1000}$$

$N = 0.299$ revolutions per second, or about 18 rpm.

$$\text{Hence Re} = \frac{1.51^2 \times 0.299 \times 1000}{0.4 \times 10^{-3}} = 1.30 \times 10^6$$

Neglecting the wall viscosity correction, $\mathrm{Nu} = 0.74 \times \left(1.3 \times 10^6\right)^{0.67} \times (1.5)^{0.33} = 10,550$

The thermal conductivity of water is about 0.66 W/m.K over this temperature range, so the inside heat transfer coefficient = 10550 × 0.66/1.51 = 4611 W/m^2K. This seems a bit high, so we might be outside the size range for which the correlation was developed. When combined with a condensing steam coefficient of ~4000 W/m^2K, this will give an overall coefficient of ~2140 W/m^2K, which is substantially higher than the estimate of 700 W/m^2K from Table 19.1. As a compromise, we can use an intermediate value, say 1000 W/m^2K, or 1 kW/m^2K.

If the initial temperature of the vessel contents is 20 °C and we use medium-pressure steam at 180 °C as heat source, we can substitute into Equation 15.32 to find the time required to reach 120 °C:

$$120 = 180 - (180 - 20)\exp\left\{-\left(\frac{1 \times 26.6}{16.75 \times 10^3 \times 4.2}\right)t\right\} \tag{15.32}$$

Hence, t = 2594 s, or 43 minutes.

According to the patent, an additional 30 minutes is required at temperature for sterilization.

Determine cool-down time

We now need to estimate the rate of cooling back to the fermentation temperature of 30 °C. Table 19.1 gives an estimate of the cooling heat transfer coefficient using an internal cooling coil to be in the range 400 to 700 W/m^2K. We can confirm this by making a layout of the cooling coil design.

The agitator diameter is 1.51 m, and we need space for baffles, so select coil diameter of 1.83 m (6 ft). If the coil is made from 1-inch tubing on a 2-inch pitch, then in 3.37 meters of filled depth, the number of coils is $3.37/(3 \times 0.0254) = 44$ coils. Each coil

has area $\pi \times 1.83 \times 0.0254 = 0.146\ m^2$, so the total coil area is $44 \times 0.146 = 6.42\ m^2$. This is not particularly large, and we could consider using a double coil if we need more area.

For heat transfer to the coil, we can use Equation 19.70f:

$$Nu = 0.87\, Re^{0.62}\, Pr^{0.33} \left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.70f}$$

Neglecting the viscosity correction, $Nu = 0.87 \times \left(1.3 \times 10^6\right)^{0.62} \times (1.5)^{0.33} = 6142$

So external heat transfer coefficient $= 6142 \times 0.66/1.51 = 2684\ W/m^2K$

Typical inside heat transfer coefficient for water in a 1-inch pipe $\sim 1000\ W/m^2K$

So overall heat transfer coefficient $= \left(\left(1000^{-1}\right) + \left(2684^{-1}\right)\right)^{-1} = 730\ W/m^2K$,

which is not too far from the value found in Table 19.1.

To solve for the cool-down time, we should make an unsteady-state energy balance on the vessel during cooling. This is more complex than Equation 15.32, as the cooling water is not at constant temperature, and the outlet temperature of the cooling water will vary as the fermenter cools down.

If the cooling water has a maximum flow rate, then we can write:

$$m_L C_p \frac{dT}{dt} = U\, A\, \Delta T_{eff} \tag{15.33}$$

where ΔT_{eff} = effective temperature difference $= \dfrac{(T - T_1) - (T - T_2)}{\ln\left(\dfrac{T - T_1}{T - T_2}\right)}$, and

$$m_w C_{pw} (T_2 - T_1) = U\, A\, \Delta T_{eff} \tag{15.34}$$

where T_1 = cooling water inlet temperature, °C, which is constant
T_2 = cooling water outlet temperature, °C, which is a function of time
m_w = mass flow rate of cooling water, kg/s
C_{pw} = specific heat capacity of cooling water = 4.2 kJ/kg°C

Equations 15.33 and 15.34 are coupled and must be solved simultaneously. This can easily be done using programs such as Mathcad or by discretizing in the space of vessel temperature, solving for T_2 and hence finding the heat transfer rate and the time to reach the next temperature. Assuming we use chilled water with a feed temperature of 10 °C and maximum velocity of 4 m/s, the cooling time required turns out to be 660 minutes or 11 hours. This is a lot less than the allowed time, so we do not need to add another coil (which would make cleaning more difficult).

Determine overall batch sequence and productivity

We now have the following overall batch sequence:

1. Fill with batch of feed medium (30 minutes, assuming same time as drain time)
2. Sterilization heat-up (45 minutes)
3. Sterilization hold (30 minutes)
4. Sterilization cool-down (11 hours)
5. Production cycle (200 hours)
6. Product drain (30 minutes)
7. Cleaning in place (4 hours)

The total nonproduction time is $0.5 + 0.75 + 0.5 + 11 + 0.5 + 4 = 17.25$ hours, which is much less than the 200 hours we allowed when we assumed 50% utilization. It might be prudent to allow some time at the end of the cool-down to confirm that the growth medium is sterile. If we allow 48 hours of hold time followed by sampling to ensure sterility, then we reduce the possibility of a contamination event and increase the nonproduction time to 66 hours. With $200/266 = 75.2\%$ utilization, we could in principle reduce the total required reactor volume to $47.6/(0.75 \times 0.75) = 84.6\ m^3$. This would allow us to reduce the number of 25-m^3 reactors to five, while still allowing for one spare fermenter in case one requires extended maintenance or manual cleaning.

Further calculations are needed to confirm that the rates of aeration and heat removal are adequate during the production cycle. The patent does not give sufficient detail to make this evaluation, so additional experimental data would be required.

15.10 Multifunctional batch reactors

In a batch process, some of the reagents are added at the start; the reaction proceeds and the compositions change with time. Additional reagents may be added as the reaction proceeds, and changes in temperature may also be made. At the end of the recipe the reaction is stopped when the required conversion has been reached and the products are withdrawn.

Batch processes are suitable for small-scale production and for processes where several different products, or grades, are to be produced in the same equipment; for instance, pigments, dyestuffs and polymers. Batch reactors are widely used in the manufacture of specialty chemicals, pharmaceuticals, and food additives, where the production volumes are relatively small, the chemistry is relatively complex, and batch integrity provides an important means of quality control. Batch processing is discussed in more detail in Section 2.3.2.

Most biochemical reactions are carried out in batch reactors, but because of the many additional constraints in biochemical reaction engineering, these are discussed separately in Section 15.9. An example of batch bioreactor design is given in Example 15.6.

Batch reactors are mainly used for liquid-phase reactions, although some reactions involving the conversion or formation of solids are carried out in batch mode. Gases may be added or removed during a batch reaction, but gas-phase reactions are almost never carried out in batch mode.

Processes that do not fit the definition of batch or continuous are often referred to as semi-continuous or semi-batch. In a semi-batch reactor, some of the products may be withdrawn as the reaction proceeds. A semi-continuous process can be one that is interrupted periodically for some purpose, for instance, for the regeneration of catalyst.

15.10.1 Design of batch reactors

Most batch reactors are stirred tanks. Mixing in stirred tanks is discussed in Section 15.5, and heat transfer to stirred vessels is addressed in Sections 15.6.2 and 19.18.

Although a batch reactor is a stirred tank and the contents are spatially well-mixed at any given time, the reactor approximates the same performance as a PFR, as back-mixing in the time dimension cannot occur.

It is not necessary to add all the reagents at the start of a batch reaction, and many batch reactions are actually operated semi-continuously, with one feed added at the start and others added during the reaction. This is almost always the case when one of the reagents is in the gas phase, in which case the gas is sparged into the reactor to maintain a constant concentration of the gas in the liquid phase.

Several reactions can be carried out in series in the same batch reactor: This is one of the advantages of batch processing. Separation steps can also be carried out between reaction steps, as discussed in the following section.

The design of a batch reactor must consider not only the rate of reaction but also the rates of all the other process steps that will be carried out in the vessel. At a minimum, these will include:

- Charging the reactor with feed, solvent, catalyst, etc.
- Heating the reactor contents to reaction temperature.
- Holding the reagents at reaction temperature for the desired residence time. In some cases, a temperature ramp profile may be applied and additional feeds may be added during the reaction.
- Cooling the reaction products to suppress reaction.
- Pumping out the reaction products to storage or downstream process operations.

The design engineer must calculate the time required for each step. The sequence of steps is often presented as a Gantt chart of the overall reaction process.

If the downstream process is operated continuously, it may make sense to operate several batch reactors, each at different points in the sequence of operations, so that at any given time one reactor is always at the pumping-out step and can feed the downstream process. This is the situation in batch fermentation of sugars to ethanol, where 6 to 12 fermenters are used to feed the continuous distillation section. Batch scheduling is discussed in Section 3.6.2 in the context of energy management: the same considerations can apply when scheduling batch reactors.

An important feature of batch plants is that they can often be used to make multiple different products in the same equipment. Multiproduct plants may use variations on the same recipe or may be scheduled to make a range of products by developing recipes that fit the plant. When an existing batch plant is evaluated (rated) for producing

a different product, the same calculations are carried out as in the design of the plant, but instead the engineer determines what production rate will be feasible within the constraints of the existing equipment.

15.10.2 Multifunctional batch reactors

It is quite common to use a batch reactor to carry out other steps in the batch processing sequence:

- The reactor can be used to heat the feeds or cool the reaction products (reactor as heater or cooler).
- At the end of a liquid–liquid reaction the products can be allowed to settle so that the liquid phases can be removed separately (reactor as decanter).
- A second solvent can be added to extract a product from the reaction mixture (reactor as extractive mixer-settler).
- The reaction mixture can be cooled or evaporated to cause crystallization of a product (reactor as crystallizer).
- A component can be added to cause a product to flocculate or precipitate from the reaction mixture (reactor as precipitator).
- The reactor can be heated to cause evaporation of a product (reactor as batch distillation still).

If other processing steps are to be carried out in the reaction vessel, the design engineer must rate the vessel for each of these steps and determine what time will be needed to achieve the desired process performance in each step. Allowance must be made for any time between steps and for time to change temperature between different operations. The total time required for all steps will determine the productivity (product capacity) of the plant. If productivity is not acceptable, the designer should consider adding another reactor or carrying out some steps in other equipment.

The design and sequencing of batch reactors and other batch operations are discussed in the books by Sharratt (1997) and Korovessi and Linninger (2005).

15.11 Computer simulation of reactors

It is not necessary to build a computer model to complete the design of a reactor. Very few industrial reactors were initially designed using computer models, although many designs have been substantially improved over the years by applying insights learned from computer simulation.

Reactor modeling is a complex, multiscale problem, spanning molecular-scale interactions, surface and diffusion effects in catalysts, mass transfer between phases, mixing and heat transfer in bulk fluids, and hydraulics of multiphase and particulate flows. These processes occur over dimensions from the order of an angstrom to the order of tens of meters. It is not usually feasible to construct a single model that treats all of these processes rigorously. Instead, reactor designers use different models to address microscopic and macroscopic phenomena.

In the early stages of design, relatively simple models can be used to estimate reactor size for the purpose of cost estimating. If the project goes ahead, it is more important to ensure that the reactor will attain the desired performance, and it may be worthwhile to build more detailed models for use in scale-up and validation of the design. It is very important to ensure that these models are fitted to realistic plant data, either from an existing full-scale plant or from a pilot plant that is able to mimic the conditions of a full-scale reactor.

Creating a model of the main process reaction is usually relatively straightforward; however, capturing the effects of side reactions, contaminants, inhibition, cell life cycle, or catalyst deactivation can be much more difficult and may require a substantial and expensive experimental program. Failure to properly include these effects may render the model inaccurate or even misleading and can lead to inferior and possibly unsafe designs. Most industrial processes use catalytic or biological routes that are sensitive to many input parameters, so it is important that these parameters are properly studied in the experimental program. The development of reactor models is discussed in all the reaction engineering textbooks cited in the bibliography. Stewart and Caracotsios (2008) give an excellent introduction to reactor modeling.

15.11.1 Commercial process simulation models

Modeling of reactors using commercial process simulation programs was discussed in Section 4.5.1, where the standard library reactor models are described. These models are adequate for determining the overall process mass and energy balance and can be very useful for calculating heats of reaction, as discussed in Section 15.3.1.

The library models in commercial process simulation programs can be used for reactor sizing if the rate of the main reaction is known or can be approximated as a simple expression under the conditions where the reactor will be operated. Instructions on how to size reactors using commercial simulation programs are given in the user manuals or online help links.

Commercial simulation programs can also be used to model more complex reactors by forming networks of simple reactors to account for mixing effects, as discussed in the next section, or by building sub-flowsheets that incorporate simple reactors and other unit operations to simulate a more complex reactor design. For example, the reactor designed in Example 15.4 and shown in Fig. 15.45 would be a single pressure vessel, but was modeled with the set of simple reactor models and other operations shown in Fig. 15.43.

15.11.2 Network models

Combinations of simple reactor models can be used to model the mixing and reaction behavior of more complex reactors. Fig. 15.55 shows some examples of simple reactor networks that can be used to model nonideal reactor behavior.

Networks of simple reactor models can also be used to determine optimum mixing patterns and heat addition profiles in real reactors, as long as a sufficiently accurate model of the reaction kinetics is available. The concept of using mixed-integer nonlinear programming (MINLP) to optimize a superstructure of simple reactor models was introduced by Kokossis and Floudas (1990) and is discussed in Section 12.11.2 as an example of the application of MINLP approaches in process synthesis. Kokossis and coworkers have extended this approach to nonisothermal, catalytic and multiphase reactors, and to reaction-separation processes. The optimal networks found from superstructure optimization can be used to infer what mixing pattern should be used in a real reactor and can lead to nonintuitive designs when the reaction mechanism is complex.

15.11.3 Hydrodynamic models

Realistic models of mixing, multiphase flow, and solids flow cannot be built using process simulation programs. To determine the effect of reactor geometry and hydraulics on the spatial variation of temperature and concentration and hence on reaction rates, it is necessary to combine a model of the reaction kinetics with a hydrodynamic model.

Hydrodynamic simulation models of any reactor geometry can be built using CFD programs. CFD programs allow the user to define a two- or three-dimensional geometry that is then discretized into a mesh of points. Boundary conditions are set for the edges of the mesh, and initial conditions are defined. The program then solves the Navier–Stokes equations for all points in the mesh in either steady-state or transient mode, and hence determines the hydraulic and mixing behavior. CFD programs were initially developed for aerospace applications, and the need for detailed models of jet engines led to the incorporation of chemical reactions into the simulation. Computational fluid dynamics programs are now routinely used for modeling reactors, as well as other process equipment; see Aglave and Eppinger (2018). Details of CFD programs, their capabilities, and their application in reaction engineering

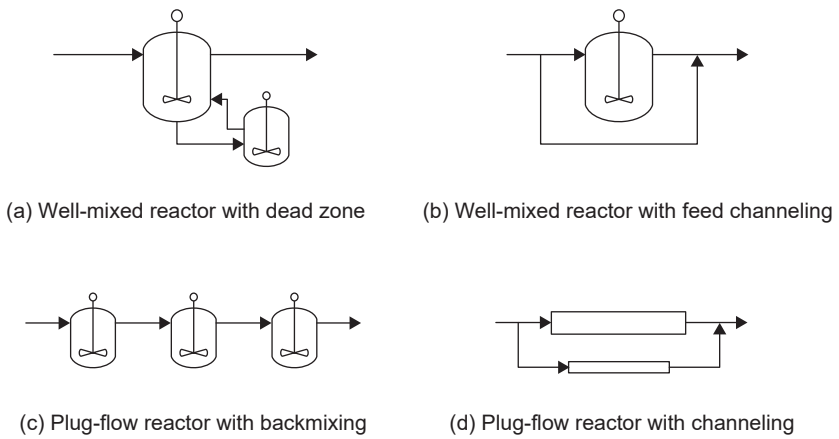


FIG. 15.55 Network models of nonideal reactors.

can be found on the websites of CFD software vendors; see, for example, http://ansys.com/ or www.cpfd-software.com/.

The development and testing of a CFD model can be expensive and time-consuming. It is essential to have good experimental or plant data to use in validating the model, so large-scale cold-flow experiments using air, water, and inert solids such as glass beads or sand are often carried out as a means of testing the hydraulic performance of the model before reaction effects are introduced.

Reaction systems that involve flowing solids present an even greater modeling challenge. Flowing solids can sometimes be treated as a pseudo-continuous fluid phase, but this approximation ignores many of the realities of particulate flow. Discrete element modeling (DEM) treats each particle separately and simulates the movement of particles and fluid through a meshed geometry. DEM methods are advancing rapidly, but at the time of writing are not yet able to solve problems with a realistic number of particles to model industrial heterogeneous catalysis. Jung et al. (2009) discuss the challenges of simulating fluidized-bed reactions using computational hydrodynamics models.

15.12 Determining actual reactor performance

The performance of full-scale commercial reactors can be difficult to predict from laboratory experiments and computer models. Many factors can affect reactor performance, particularly for catalytic or biological processes. If the experimental system does not carefully control these factors and provide a realistic model of the mixing and heat transfer that will be achieved in the real reactor, different performance may be obtained when the reaction is carried out at full scale.

Experience with similar reaction systems is usually the best way to ensure successful scale-up. The design of experimental reactors and scale-up are discussed by Rase (1977) and Bisio and Kabel (1985).

In most cases, any new reactor design will require testing and validation at the pilot-plant scale before a full-scale unit is built. This section discusses some of the important issues to address and techniques that can be deployed when determining whether a proposed reactor design will work as intended at full scale.

15.12.1 Measuring experimental reactor output

For a laboratory or pilot-plant reactor to successfully model the behavior of a full-scale reactor, the following factors must be considered:

- **Mixing pattern:** The mixing pattern in the experimental reactor should model that of the real reactor as closely as possible. This does not mean that the experimental reactor must be a smaller version of the commercial-scale reactor. The reaction engineer must give some thought as to whether to mix the feeds before heating, mix them inside the reactor itself, etc. At the small scale, mixing will generally be quicker than at the large scale, but there is a greater chance of channeling, bypassing, wall effects, and laminar flow effects.
- **Material balance**: It is very important to properly close a material balance across the experimental reactor for every data point. This is not as easy as it sounds, particularly when some products are in the vapor phase. Vaporized products must be collected using vent condensers or gas-phase sampling, and the composition of the vapor phase must be tied to the composition of the liquid phase at the time the sample was taken. The research engineer should be able to complete a material balance for every element (C, H, O, etc.), as well as an overall material balance. If an element cannot be materially balanced, that can be an indication of poor test methodology or of accumulation of species in the reactor or on the catalyst. In some cases, as in the growth of microorganisms, the accumulation is desired, and it is important to know uptake rates of feed species such as minerals to determine the required rates for processing.
- **Energy balance and temperature profile:** Small-scale reactors are difficult to operate adiabatically, as the surface area—to—volume ratio is large and so heat is easily lost to (or gained from) the environment. When a reaction is run at or near ambient conditions, the temperature must be carefully controlled to eliminate diurnal or seasonal variations in temperature. Reactors should be well insulated and should be instrumented to allow measurement of the temperature in multiple locations so that the temperature profile is properly understood. If possible, the temperature profile in the experimental reactor should match that expected in the commercial reactor, and multiple heating zones or reaction zones may need to be used to correctly model the commercial reactor temperature pattern.
- **Mass transfer:** Mass transfer rates between phases or inside solid catalysts can govern the overall rate of reaction. If mass transfer is likely to be limiting at the commercial scale, the experimental reactor should allow

measurement of the mass transfer rate or allow reaction kinetics and mass transfer to be de-confounded so that models can be developed that predict performance at full scale.

- **Feed composition:** Whenever possible, the experimental feed should be the same as the feed that will be used in the commercial plant. Laboratory-grade chemicals will have higher purity than commercial grades and are less likely to contain contaminants that may play an important role in reactor performance. Experiments using pure model compounds may be useful for determining reaction mechanisms, but can overlook significant effects such as catalyst inhibition. It may not always be possible to use the commercial feed, for example, if the plant is to be fed from an upstream process that has not yet been built; however, when the real feed is not available, the test program should err on the side of caution by dosing potential contaminants into the model feed to understand their impact.
- **Recycle structure:** If the process uses a recycle, then the pilot plant or laboratory reactor should also be designed to incorporate a recycle. Trace components that are formed in the reaction can accumulate in recycle streams and affect reactor performance. It is important to identify these effects experimentally before scale-up so that the correct reactor performance is predicted. In some cases, the process may even need to be modified by adding a separation process to control the recycle composition.
- **Steady state:** The experimental design must allow sufficient time for the reactor to reach steady-state performance if a continuous system is used. This requires achieving thermal steady state, stable conversion, and stable concentration of components in recycle streams. If process conditions are modified, the system must again return to steady state before data can be collected.
- **Catalyst or cell age:** For catalytic and biological processes, the behavior of the catalyst or cell population can vary with time. Catalysts can lose their activity due to inhibition, coking, or damage suffered during regeneration cycles. Microorganisms may pass through many generations during a processing run (even in a batch process) and consequently can experience evolutionary effects that change productivity. The experimental design must allow for these effects and ensure that the experimental run length is adequate to predict reactor performance over the anticipated process time between catalyst or cell culture replacement.

15.12.2 Measuring commercial reactor behavior

It is much more difficult to carry out experiments using large-scale commercial reactors, as they are not as highly instrumented as pilot plants, and the primary imperative for operators is to maintain safe and steady operation at optimal conditions to generate revenue. Nonetheless, data taken from operating units can play an important role in reactor design and development. The techniques used to collect data from commercial plant must cause no interruption to normal operation, require no shutdown or plant modification, and cause no hazard to workers or the plant.

Tracer studies

Experiments using tracer molecules can be used to determine the residence time distribution in a real reactor. The most common noninvasive approach is to use a radioactive tracer species that has a half-life that is long enough for detection, but short enough that there will be no residual radiation in the plant or products. The species must also be chosen so that the radioactive decay products are not toxic, reactive, or otherwise problematic for the reactor or downstream process operations.

In a tracer experiment, detectors are positioned around the reactor or in downstream piping. The tracer molecule is injected upstream of the reactor, usually into one of the feed lines, and the signal at each detector is then logged as a function of time. The signal strength gives a measure of the concentration of tracer passing that point, and hence allows the residence time distribution to be constructed.

Tracer studies provide insight into the distribution of residence times and can be very useful in identifying deviations from the expected mixing pattern. Tracer experiments can identify channeling, bypassing, unwanted backmixing, and the presence of dead zones. The use of tracer studies on an existing reactor can help suggest modifications to reactor geometry and internals that would improve the performance of the existing reactor or of future reactors in a new design. Examples of commercial applications of tracer studies can be found from vendor websites; see, for example, www.tracerco.com.

Residence time distributions measured from real plant can be used to construct models of commercial reactors that predict plant performance better than idealized reactor models. The use of networks of simple models to fit real reactor residence time distributions is discussed in Section 15.11.2.

Reactor tomography

Tomography is imaging of the internal structure of objects by carrying out multiple sectional scans using penetrating radiation. Tomography can be applied to reactors using x-rays or gamma rays, depending on the reactor wall thickness, and can reveal regions of local high or low density inside the reactor. Tomography studies can be carried out while the reactor is in operation at design conditions, as the technique is noninvasive.

Tomography studies are very useful for understanding particulate and multiphase flows. Tomography results can be used to validate CFD models, which can then be used to propose improvements to reactor internals and other features of the design. Tomographic studies of existing commercial-scale reactors can be quite valuable as a means of validating models that can then be used to design novel reactors. An example of the application of tomography to FCC is given by Wolschlag and Couch (2010).

15.13 Safety considerations in reactor design

The reactor is often the highest temperature point in the process. It is also where reactive species are brought together and where heat of reaction may be released. The residence time required for reactors can be long compared with processing times in other operations, so the inventory of chemicals in the reactor can be relatively high. All of these factors make reactors hazardous and require the design engineer to pay particular attention to safety when developing a reactor design.

15.13.1 Inherently safer design principles applied to reactors

The concept of inherently safer design was introduced in Section 10.1.3. The basic principle of inherently safer design is to remove or reduce process hazards and thereby reduce the impact of undesired or unforeseen events. Inherently safer design methods are complementary to adding passive, active, and procedural layers of protection to the design and do not guarantee a safe process or remove the need for extrinsic safety systems. Inherently safer design methods should be applied at an early stage in the design as part of good engineering practice and is not something that can be added later by a specialist in process safety.

Guidelines for inherently safer design have been articulated by Kletz and others and are set out in the books by Kletz and Amyotte (2010), CCPS (2008), Cameron and Raman (2005), Mannan (2012), and Crowl and Louvar (2011). The core principles are to eliminate hazardous conditions (*eliminate*), reduce inventories (*minimize*), use less hazardous materials (*substitute*), operate under less hazardous conditions (*moderate*), and eliminate complexity so that errors are less likely to occur (*simplify*). It should be noted that often one of these principles will have to be traded off against another. For example, moderating reaction conditions by operating at lower temperature will lead to a lower reaction rate and hence require a longer residence time and higher inventory.

Table 15.16 gives some examples of application of inherently safer design principles in reactor design and points out some of the possible trade-offs that may be introduced. It is important to consider potential trade-offs so that the hazard is truly reduced and not just shifted elsewhere in the process, or even made worse. The list in Table 15.16 is not exhaustive, and the reader should refer to the books cited above for additional examples.

15.13.2 Designing for exothermic reactions

Exothermic reactions are particularly hazardous because heat released by the reaction can increase the temperature of the reaction mixture, thereby increasing the reaction rate, releasing more heat, and ultimately allowing the reaction to run away. When an exothermic reaction is unavoidable, the designer must ensure that the temperature change of the reaction mixture can be carefully controlled and that the reaction can quickly be shut down if temperature control is lost.

The use of solvent or inert diluent allows moderation of the temperature change by increasing the heat capacity flow rate (thermal mass) of the mixture relative to the rate of heat release per unit mass of mixture. Provision can be made to flood the reactor with cold diluent or solvent as an emergency response if the temperature exceeds a critical limit.

If a cooling system is used, it should be designed so that it has the capacity to handle the rate of heat release at the maximum temperature conditions expected in operation. The cooling system should then be able to return the process to the desired temperature range if the maximum temperature is reached and the cooling system is operational.

TABLE 15.16 Some applications of inherently safer design approaches in reactor design

Inherently safer design principle	Reactor application	Rationale	Possible trade-offs
Minimize	Use continuous processing instead of batch processing	Pipe reactor has less inventory than a tank and is easier to close off.	Fed-batch system may be safer if reaction rate can be limited by carefully controlling addition of one component.
Minimize	Use large number of small reactors (process miniaturization)	Impact from a hazardous event in one reactor is reduced.	Higher probability of a hazardous event occurring. More complex system. Higher production costs.
Minimize	Use more active catalyst	More active catalyst allows smaller reactor volume.	Higher rate of heat release if reaction is exothermic.
Minimize	Combine reaction and separation, as in reactive distillation	Fewer process vessels.	Total liquid inventory may increase. Conditions that are effective for separation may lead to longer residence times for reaction.
Minimize	Operate at higher conversion	Reduces recycle of material, hence inventory of unconverted feed in separation section.	Usually leads to poor selectivity, which may actually increase complexity of the separation section. Inventories of by-products may increase.
Minimize	Improve mixing	Reduces reaction time, hence inventory.	Higher rate of heat release if reaction is exothermic.
Substitute	Use nonflammable solvent instead of flammable	Nonflammable solvent cannot cause a fire.	Many nonflammable solvents are halogenated compounds that have high global warming potential.
Substitute	Use biological processing route	Biological routes are carried out in aqueous media at ambient conditions, therefore less hazardous.	Much larger reactors. Increase in wastewater production.
Substitute	Use different chemical route	An alternative chemical route may be available that avoids the use of explosive or highly toxic compounds.	
Substitute	Use steam as heat source instead of fired heat or electric heaters	Steam heating is intrinsically limited to the temperature of the steam; therefore is safer than electric heaters or fired heaters.	Harder to reach high temperatures; therefore may have the effect of reducing reaction rate. May require high-pressure steam or introduce possibility of water leaking into process.
Moderate	Operate at lower temperature	Leaking material will be further from flash point, autoignition temperature. Liquids below atmospheric boiling point are less likely to suffer boiling liquid expanding vapor explosion (BLEVE).	Reaction rate is reduced, increasing residence time and inventory. Reactor is larger and more expensive.
Moderate	Operate at lower pressure	Reduced consequences of overpressure, reduced inventory.	Lower reaction rates, so longer residence times. Much larger vessels are required.
Moderate	Operate at higher dilution	Reduced reaction intensity, less change in temperature due to heat of reaction.	Additional complexity due to additional species (solvent, diluent) introduced into the process, possibly requiring additional separations or other processing.
Simplify	Eliminate discontinuous operations	Failure of a switching valve could cause a hazardous situation.	
Simplify	Carry out reaction inside heat exchanger	Fewer vessels, lower inventory.	Possibility of leaks from process to utility or vice-versa.

Shutting off the feed to an exothermic reaction is not always a safe strategy for preventing reaction runaway. If feed-effluent heat exchange was used, then shutting off the feed reduces cooling of the reactor product and allows overheated product to enter downstream operations. If the reactor relied upon cold feed to provide some of the cooling requirement, then shutting off the feed can reduce the rate of cooling and worsen the runaway condition. It may be more effective to shut off only one of the reagents or to substitute a reagent with a cold inert material that has the same cooling effect but no reaction.

The consequences of loss of cooling, loss of diluent, and reactor runaway should always be considered in hazard and operability studies and as pressure relief scenarios whenever an exothermic reaction is used. Additional safety systems may need to be added to the process, and the safety integrity level (SIL) of safety instrumented systems associated with the reactor may need to be increased.

15.13.3 Venting and relief of reactive systems

The contents of a reactor can continue to react if containment is lost or if an overpressure event causes discharge of material into the pressure relief system. The presence of reaction substantially complicates the design of the pressure relief device and the downstream relief system.

In 1976 a consortium of 29 companies formed the Design Institute for Emergency Relief Systems (DIERS) under the auspices of the American Institute of Chemical Engineers (AIChE). The DIERS consortium developed design methods and software for designing relief systems for runaway reactions. At the time of writing, the DIERS methodology is maintained and updated by a users group drawn from 160 companies. Details of the DIERS consortium and their publications can be found via the AIChE website, www.aiche.org.

When a runaway reaction could occur, the design of the relief system should follow the guidelines specified in the DIERS methodology. The reactor design team must have a very good understanding of the reaction mechanism and kinetics, including the role of any trace compounds that may act as catalysts or free radical promoters or might otherwise accelerate the reaction. The experiments to collect kinetics data for exothermic reactions can also be hazardous and must be carefully planned and executed. They are often subcontracted to companies that specialize in this area. Additional information on designing relief systems for reactive mixtures is given in the articles by Fauske (2000) and Melhem and Powell (2005).

15.14 Capital cost of reactors

Most reactors are designed to be operated under conditions that cause the reaction vessel to be classified as a pressure vessel. Once the reactor dimensions have been determined following the procedure given in Section 15.2.1 and the other methods given in this chapter, the pressure vessel design methods given in Chapter 14 can be used to estimate the wall thickness and hence determine the capital cost. Additional costs may need to be added to cover the cost of reactor internals or other ancillary equipment such as agitators. This procedure was illustrated in Example 15.4.

The costs of jacketed stirred-tank reactors are not easily addressed using simple pressure vessel cost correlations. A substantial part of the cost is in the construction of the vessel jacket. In some cases, the jacket can cause the wall of the reaction vessel to be in compression, requiring a more complex analysis of the pressure vessel wall thickness. Instead, a commonly used method in preliminary cost estimating is to use a different correlation for jacketed stirred tanks operated at low pressures (below about 20 bar). Table 7.2 gives such correlations for plain and glass-lined stirred vessels.

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15.16 Nomenclature

		Dimensions in MLT
A	Area	$\mathbf{L}^2$
a	Interfacial area per unit volume	$\mathbf{L}^{-1}$
a_i	activity of component i	—
b	Index in equation 15.16	—
C_A	Concentration of A in the liquid phase	$\mathbf{ML}^{-3}$
$C_{A,i}$	Concentration of A in the liquid at the interface	$\mathbf{ML}^{-3}$
$C_{A,bulk}$	Concentration of A in the bulk liquid	$\mathbf{ML}^{-3}$
C_B	Concentration of B in the liquid phase	$\mathbf{ML}^{-3}$
C_p	Specific heat capacity	$\mathbf{L}^2\mathbf{T}^{-2}\,\boldsymbol{\theta}^{-1}$
C_{pw}	Specific heat capacity of cooling water	$\mathbf{L}^2\mathbf{T}^{-2}\,\boldsymbol{\theta}^{-1}$
C	Index in equation 15.16	—
D	Diffusivity	$\mathbf{L}^2\mathbf{T}^{-1}$
D	Impeller diameter (Fig. 15.15)	**L**
D_A	Diffusivity of component A	$\mathbf{L}^2\mathbf{T}^{-1}$
D_i	Vessel internal diameter	**L**
D_L	Liquid phase diffusivity	$\mathbf{L}^2\mathbf{T}^{-1}$
$\mathrm{D_T}$	Tank diameter (Fig. 15.15)	**L**
D_v	Vapor phase diffusivity	$\mathbf{L}^2\mathbf{T}^{-1}$
d_a	Agitator diameter	**L**
d_p	Particle diameter	**L**
d_t	Tube diameter	**L**
E	Welded joint efficiency	—
ΔG	Change in Gibbs free energy	$\mathbf{L}^2\mathbf{T}^{-2}$
g	Gravitational acceleration	$\mathbf{LT}^{-2}$
ΔH_{rT}	Heat of reaction at temperature T	$\mathbf{L}^2\mathbf{T}^{-2}$
$\Delta H_{\mathrm{react.}}$	Enthalpy change to bring reactants to standard temperature	$\mathbf{L}^2\mathbf{T}^{-2}$
$\Delta H_{\mathrm{prod.}}$	Enthalpy change to bring products to reaction temperature	$\mathbf{L}^2\mathbf{T}^{-2}$
h_i	Tube-side heat transfer coefficient for a packed tube	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
K	Reaction equilibrium constant	units vary
K	Constant in equation 15.16	—
k	Mass transfer coefficient	$\mathbf{LT}^{-1}$
k_L	Mass transfer coefficient in liquid phase	$\mathbf{LT}^{-1}$
k_1	First order rate constant	$\mathbf{T}^{-1}$
k_2	Second order rate constant	$\mathbf{M}^{-1}\mathbf{L}^3\mathbf{T}^{-1}$
L_b	Length of a packed bed of solids	**L**
M_i	Molecular mass of component i	**M**

		Dimensions in MLT
M_{in}	Molar flow rate of any component into the reactor	$\mathbf{MT}^{-1}$
M_{out}	Molar flow rate of any component out of the reactor	$\mathbf{MT}^{-1}$
M_w	Molecular mass of solvent	$\mathbf{M}$
m	Mass flow rate	$\mathbf{MT}^{-1}$
m_i	Rate of consumption of substrate i to maintain cell life	$\mathbf{T}^{-1}$
m_L	Mass of liquid in vessel	$\mathbf{M}$
m_w	Mass flow rate of cooling water	$\mathbf{MT}^{-1}$
N	Agitator speed	$\mathbf{T}^{-1}$
n	Total number of components	—
P	Pressure	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
P_a	Agitator power input	$\mathbf{ML}^{2}\mathbf{T}^{-3}$
P_i	Internal pressure	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
ΔP	Pressure differential (pressure drop)	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
P	Partial pressure of adsorbed component	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
p	Agitator blade pitch (Fig. 15.15)	$\mathbf{L}$
Q	Gas volumetric flow rate	$\mathbf{L}^{3}\mathbf{T}^{-1}$
$\mathbf{R}$	Universal gas constant	$\mathbf{L}^{2}\mathbf{T}^{-2}\boldsymbol{\theta}^{-1}$
$\Re$	Rate of reaction	$\mathbf{ML}^{-3}\mathbf{T}^{-1}$
S	Maximum allowable stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
s_i	Concentration of substrate i	$\mathbf{ML}^{-3}$
T	Temperature	$\boldsymbol{\theta}$
T_o	Initial temperature	$\boldsymbol{\theta}$
T_w	Wall temperature	$\boldsymbol{\theta}$
T_1	Cooling water inlet temperature	$\boldsymbol{\theta}$
T_2	Cooling water outlet temperature	$\boldsymbol{\theta}$
ΔT_{eff}	Effective temperature difference	$\boldsymbol{\theta}$
t	Time	$\mathbf{T}$
t	Pressure vessel wall thickness (Equation 14.13)	$\mathbf{L}$
U	Overall heat transfer coefficient	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
u	Superficial velocity	$\mathbf{LT}^{-1}$
u_p	Particle velocity relative to the fluid	$\mathbf{LT}^{-1}$
V	Reactor volume	$\mathbf{L}^{3}$
V_{liq}	Liquid volume	$\mathbf{L}^{3}$
V_m	Molar volume of the solute at its boiling point	$\mathbf{M}^{-1}\mathbf{L}^{3}$
v_i	Special diffusion volume coefficient in Equation 15.9	$\mathbf{L}^{3}$
w	Impeller width (Fig. 15.16)	$\mathbf{L}$
x	Concentration of cells	$\mathbf{ML}^{-3}$
Y_i	Yield of new cells on substrate i	—
α_j	stoichiometric coefficient of component i	—
δ	Thickness of boundary layer	$\mathbf{L}$

		Dimensions in MLT
ε	Bed void fraction	—
λ_f	Fluid thermal conductivity	$\mathbf{MLT^{-3}\theta^{-1}}$
μ	Fluid viscosity	$\mathbf{ML^{-1}T^{-1}}$
μ_g	Growth rate	$\mathbf{T^{-1}}$
ρ	Liquid density	$\mathbf{ML^{-3}}$
ρ_f	Fluid density	$\mathbf{ML^{-3}}$
τ	Residence time	$\mathbf{T}$
Φ	Solvent association factor	—
Dimensionless numbers		
Fr	Froude number	
Ha	Hatta number	
N_p	Power number, defined by Equation 15.16	
Pr	Prandtl number	
Re	Reynolds number	
Sc	Schmidt number	
Sh	Sherwood number	

15.17 Problems

15.1. Acrolein ($H_2C{=}CHCHO$) is made by selective oxidation of propylene at 2 bar, 350 °C using a molybdenum, iron, and bismuth catalyst on a silica support. The reactor yields based on propylene are 85% acrolein, 10% acrylic acid, and 5% light by-products. The light by-products are mostly acetaldehyde, but for the purpose of this problem, it can be assumed that the yield is 85% acrolein and 15% acrylic acid. The feed to the reactor on a volume percent basis is propylene 6%, propane 28%, steam 6%, oxygen 11%, and balance nitrogen. Estimate the reactor cooling requirement for a plant that produces 20,000 metric tons per year (20 kt/y) of acrolein if the reactor is operated isothermally.

15.2. Styrene can be made by catalytic dehydrogenation of ethylbenzene. The reaction is usually carried out in the presence of steam, which acts as a heat carrier and reduces coking on the catalyst. If a mixture of steam and ethylbenzene is fed to an adiabatic reactor at 2 bar, 640 °C, estimate the equilibrium conversion and outlet temperature as a function of the ratio of steam to ethylbenzene. What ratio would you recommend using in practice?

15.3. Aniline is produced by the hydrogenation of nitrobenzene. The reaction takes place in a fluidized bed reactor operating at 270 °C and 20 bar. The excess heat of reaction is removed by a heat transfer fluid passing through tubes in the fluidized bed. Nitrobenzene vapor and hydrogen enter the reactor at a temperature of 260 °C. A typical reactor off-gas composition, mole percent, is: aniline 10.73, cyclo-hexylamine 0.11, water 21.68, nitrobenzene 0.45, hydrogen 63.67, and inerts (take as nitrogen) 3.66. Estimate the heat removed by the heat transfer fluid for a feed rate of nitrobenzene to the reactor of 2500 kg/h.

15.4. Hydrogen chloride is produced by burning chlorine with an excess of hydrogen. The reaction is highly exothermic and reaches equilibrium quite rapidly. The equilibrium mixture contains approximately 4% free chlorine, but this is rapidly combined with the excess hydrogen as the mixture is cooled. Below 200 °C the conversion of chlorine is essentially complete.
The burner is fitted with a cooling jacket, which cools the exit gases to 200 °C. The gases are further cooled to 50 °C in an external heat exchanger.

For a production rate of 10,000 tons per year of hydrogen chloride, calculate the heat removed by the burner jacket and the heat removed in the external cooler. Take the excess hydrogen as 1% over stoichiometric. The hydrogen supply contains 5% inerts (take as nitrogen) and is fed to the burner at 25 °C. The chlorine is essentially pure and is fed to the burner as a saturated vapor. The burner operates at 1.5 bar.

15.5. A 100-liter fed-batch fermenter was successfully operated for 200 h using an aeration rate of 14 l/s and a 5 W agitator. It is proposed to scale the fermentation up to 10,000 liters. What agitator power consumption is required?

15.6. Isophthalic acid (IPA, formula HOOC−C_6H_4−COOH) is made by oxidation of *m*-xylene with air. The reaction is carried out in acetic acid solvent at about 200 °C using a cobalt−manganese catalyst promoted by bromine. Acetic acid is boiled off, condensed, and returned to the reactor to remove the heat of reaction, and the reactor pressure is set to allow an adequate evaporation rate of acetic acid. IPA is not soluble in acetic acid, so the product crystallizes and a slurry can be removed from the base of the reactor for product recovery. Design and size a reactor system for production of 25,000 metric tons per year of IPA.

15.7. In the acrolein process introduced in Problem 15.1, the catalyst is packed in tubes and the reactor is cooled using a circulating molten salt. The molten salt rejects heat to boiling steam in a similar arrangement to that shown for phthallic anhydride in Fig. 15.25. The required gas hourly space velocity is 200 standard liters (at STP)/liter.h. Design and size a reactor to produce 20 kt/y of acrolein.

15.8. Acetylene is formed as a by-product in the manufacture of ethylene. It is removed by selective hydrogenation using noble metal catalysts (see, for example, US 7,453,017). A particular catalyst achieves 90% acetylene saturation with 50% hydrogen selectivity for acetylene at a weight hourly space velocity of 800 h^{-1} based on ethylene. Design a reactor to remove 1% acetylene from ethylene in a plant that produces 1.5 million metric tons per year of ethylene using this catalyst.

15.9. It is proposed to sterilize the growth medium fed to a continuous bioreactor by holding it at either 120 °C for 15 minutes or at 140 °C for 3 minutes. The feed must contain 12 mg/l of vitamin C and 0.3 mg/l of thiamin. Leskova et al. (2006) give the following first-order rate constants for thermal decomposition of these vitamins:

Vitamin	k_o (s^{-1})	E_a (kJ/mol)
Ascorbic acid (vitamin C)	3.6×10^2	46
Thiamin (vitamin B1)	1.88×10^9	97

Where the first-order rate constant $k_1 = k_o \exp(-E_a/\mathbf{R}T)$
Determine the amount of each vitamin that must be added to the feed before sterilization for each heat treatment. Which sterilization treatment do you recommend?

15.10. The reaction of Example 15.5 can be carried out in a heat exchanger reactor, using boiling water as coolant. Design and size a reactor to produce 40,000 metric tons per year of cyclohexane.

15.11. The fermentation of cane sugar to ethanol was introduced in Problem 4.3, and typical yields were given. Design the reactor system for a plant that produces 500,000 metric tons per year of ethanol using continuous fermentation.

15.12. The batch fermentation of glucose to glutamic acid using *Brevibacterium divaricatum* is described in detail in US patent 2,978,384. In Example I in the patent a 10.5 wt% glucose feed was fermented for 72 hours at 30 °C, giving 33.5 wt% glutamic acid yield on glucose. What annual production of glutamic acid can be achieved in a batch fermentation plant that has four 10,000-liter reactors? The reactors have jackets that can be used for steam heating or water cooling, but no internal coils.

CHAPTER

16

Separation of fluids

KEY LEARNING OBJECTIVES

- How to separate mixtures of gases
- How to separate droplets of liquid from a gas or second liquid phase
- How to separate dissolved components from liquid mixtures
- Design of separations using adsorption, membranes, knockout pots, decanters, coalescers, ion exchange, reverse osmosis, and chromatography

16.1 Introduction

Separation processes play an important role in all of the process industries. In addition to recovering components from reactor products, separations are used to purify feeds, products, and recycle streams and to treat effluent streams to meet environmental regulations.

Most separation processes are based on the concept of partitioning a component between two phases that can be physically separated. In some cases, two or more phases are formed from the process stream, for example, in condensation or evaporation, whereas in other cases an additional separating agent is introduced, as in adsorption, chromatography, or liquid–liquid extraction.

This chapter and the following chapter cover fluid-phase separations. Chapter 16 discusses separation of gas mixtures, physical separation of vapor–liquid and liquid–liquid mixtures, and recovery of dissolved components from liquids. Chapter 17 focuses on separations that use multistage contacting columns, particularly vapor–liquid separations such as distillation, absorption, and stripping, which are the most widely used separation techniques in the chemical process industries. Separations that involve the formation or recovery of a flowing solid phase are intrinsically linked to solids forming, sizing, and handling processes that are described in the chapter on solids processing; see Chapter 18.

Many of the separation techniques described in this chapter require the use of proprietary separating agents or equipment, and so would normally be designed in consultation with a technology vendor. Sufficient information is given here for a design engineer to make a preliminary design and estimate the critical sizing parameters that are needed to generate a Class 4 or Class 5 cost estimate using commercial costing software; however, a design selection should not be made without obtaining a more realistic estimate from discussion with a vendor. Contact information for technology and equipment suppliers can easily be obtained by searching the Internet.

Several excellent textbooks provide an overview of separations processes, discuss the underlying physical phenomena, and derive the design equations. Chhabra and Gurappa (2019) and McCabe et al. (2004) are particularly recommended. Descriptions and illustrations of most of the equipment used can also be found in various handbooks:

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Green and Southard (2018), Schweitzer (1997), and Couper et al. (2012). Other texts that focus on specific unit operations are referenced in the relevant sections. Equipment manufacturers' advertisements in the technical press and online should also be studied. Manufacturer's websites are usually easily located online and often provide details of equipment construction, standard sizes, available metallurgies, specification sheets, and performance information. It is worthwhile building up a personal file of vendors' websites that have good information to eliminate repeated searching.

16.2 Gas–gas separations

Separation of gaseous or vapor components from the gas phase is important in many industrial processes:

1. Preparation of high-purity industrial gases such as oxygen, nitrogen, argon, neon, hydrogen, etc.
2. Purification of natural gas to meet specifications for pipelines and liquefaction plants.
3. Treatment of process gases to prevent accumulation of contaminants in recycles or to protect catalysts.
4. Removal of pollutants from vent gases to meet legislative requirements.
5. Drying and purification of air for use in sterile dryers, clean rooms, as instrument air, etc.

Bulk removal of condensable vapor components from a gas can usually be accomplished by cooling and condensation; see Section 19.10; however, even refrigerated condensers seldom give adequate recovery of the vapor, and additional separation is usually needed to meet product gas or vent gas specifications.

16.2.1 Adsorption

Adsorption is probably the most widely used method in gas separation. Adsorption can be expensive for bulk separation of large quantities of gas, but it has the advantage of allowing very high gas purities or high recoveries of contaminants to be achieved.

The basic principle of adsorption is to exploit differences in the strength of interaction between different species in the gas phase and the surface of a solid known as a sorbent or adsorbent. If one species is more strongly adsorbed, then it accumulates on the sorbent as the gas passes through a bed of sorbent, and hence is removed from the gas phase. If the gas flows down through the sorbent bed, as shown in Fig. 16.1(a), then it continues to contact fresh sorbent and all of the adsorbed component is removed, giving a purified gas. As the sorbent accumulates the adsorbed component, it eventually becomes saturated and can adsorb no more. A concentration profile is thus established in the sorbent bed (see Fig. 16.1b). The concentration profile moves down through the bed until it reaches the bottom, at which point *breakthrough* of the adsorbed component occurs and the concentration in the exit gas begins to rise. Breakthrough occurs at the time labeled t_B in Fig. 16.1. The thermodynamics and kinetics of adsorption that lead to the formation of the concentration profiles shown in Fig. 16.1(b) are discussed in detail in the books by Ruthven (1984), Yang (1997), Chhabra and Gurappa (2019), and Ruthven et al. (1993). An introduction to adsorption design is given in the article by Gabelman (2017). Adsorption is also covered in the books by Suzuki (1990) and Crittenden and Thomas (1998).

Irreversible adsorption

When adsorption is used to remove a low level of a contaminant from a gas stream, a sorbent can be selected that reacts irreversibly with the contaminant. In this case, the process is termed irreversible adsorption, and the adsorption vessel is sometimes referred to as a guard bed. An example of irreversible adsorption is the use of zinc or copper oxide to remove trace amounts of hydrogen sulfide from natural gas and petrochemical processes.

When a bed of irreversible sorbent becomes saturated, it must be replaced. A common arrangement is to use two beds in parallel, with one in service and the other isolated to allow for sorbent change-out (Fig. 16.2). This scheme is simple, but can be wasteful of sorbent, as the bed must usually be replaced before breakthrough occurs.

An alternative is to use a *lead–lag* arrangement (Fig. 16.3). In this flow scheme, the gas normally flows through both beds in series, as illustrated in the figure. When the first (lead) bed becomes saturated and breakthrough occurs, then the second (lag) bed removes the contaminant, so there is no breakthrough to the product gas. The first bed is then removed from service for sorbent change-out while the feed gas flows through the second bed alone. The first bed is then placed back into service and becomes the lag bed, while the second bed now operates as lead bed. This arrangement allows the sorbent to be completely used up and reduces spent sorbent waste disposal costs.

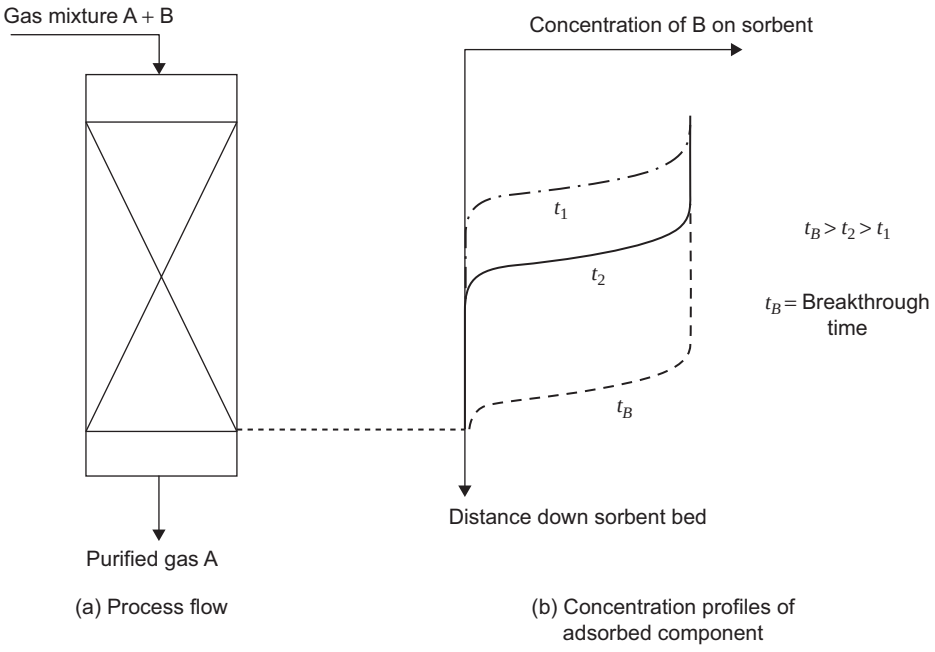


FIG. 16.1 Adsorption.

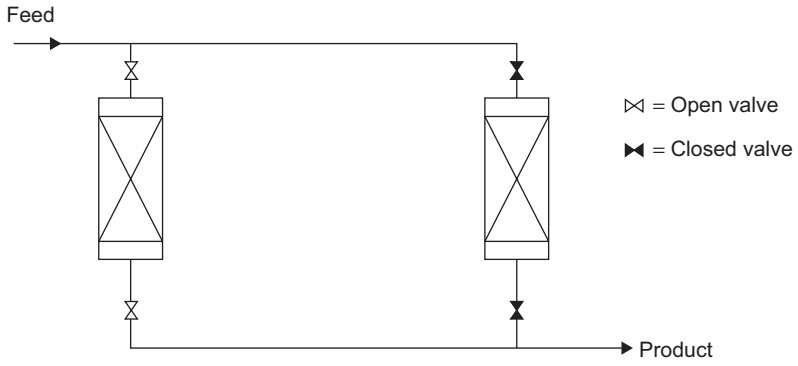


FIG. 16.2 Parallel flow through guard beds.

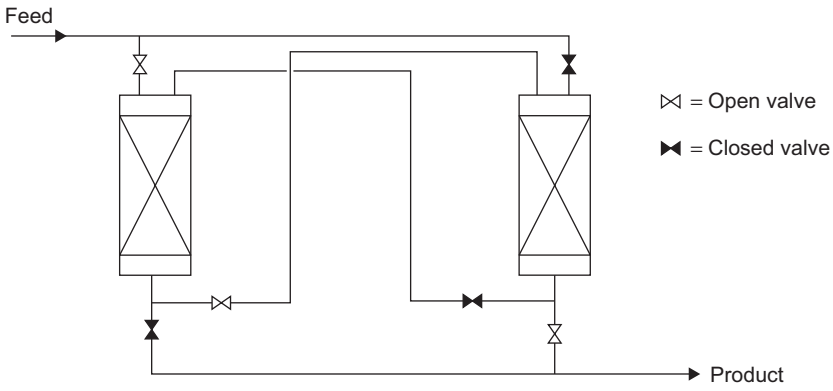


FIG. 16.3 Lead–lag guard beds.

The sorbents for irreversible adsorption are usually cheap, but the process can only be justified when the amount of contaminant removed is small, because the inconvenience and labor costs of changing out sorbent and the costs of waste disposal must also be taken into account.

Reversible adsorption

In most cases, irreversible adsorption is not practical, as the adsorbed component either has high flow rate or is desired as a product. When the bed reaches or nears breakthrough, it must be taken out of process service so that the sorbent can be regenerated and the adsorbed components recovered. Multiple beds are usually used, with an arrangement of isolation valves that allows the beds to be sequenced so that a fresh bed of sorbent is brought into service whenever a bed is switched to regeneration.

Regeneration of the sorbent is usually carried out by increasing temperature or reducing pressure to give a lower equilibrium concentration of the adsorbed component on the solid surface. The equilibrium between the partial pressure of a component in the vapor phase and the adsorbent loading, expressed as grams of adsorbed material per gram of adsorbent, can be plotted at constant temperature as an isotherm (Fig. 16.4). Various expressions can be used to model isotherms, but for design purposes they can usually be fitted with an equation of the form:

$$m = kp^n \tag{16.1}$$

where m = adsorbent loading, g/g adsorbent
k = equilibrium constant
p = partial pressure of adsorbed component
n = exponent

Fig. 16.4 shows isotherms at two temperatures, T_2 and T_1, where T_2 is greater than T_1. It can be seen from the figure that a change in adsorbent loading from m_1 to m_2 could be accomplished either by decreasing the partial pressure from p_1 to p_2 at constant temperature T_1, or by increasing temperature from T_1 to T_2 at constant pressure p_1. Cycling the bed over a range of temperature or pressure thus allows material to be adsorbed under process conditions and then recovered from the bed under regeneration conditions.

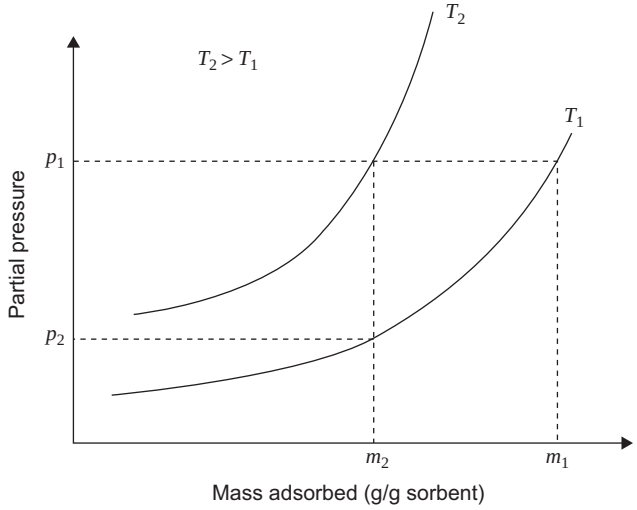


FIG. 16.4 Adsorption isotherms.

Pressure swing adsorption

When the bed is regenerated by reducing pressure, the process is known as pressure swing adsorption (PSA). Pressure swing adsorption processes are nominally isothermal, although heat of adsorption and desorption effects must be allowed for in the design. Because the process is not limited by heat transfer rates, very rapid cycles as short as a few minutes can be used. Rapid cycling gives efficient use of adsorbent and leads to smaller vessel sizes and lower capital cost.

If the process feed is under high pressure, then carrying out the regeneration at or near atmospheric pressure may be adequate. Alternatively, a vacuum pump can be used to generate a lower pressure for regeneration, in which case the process is known as vacuum swing adsorption (VSA or VPSA).

A small flow of sweep gas is usually passed through the bed during regeneration to promote desorption and clear away the desorbed components. The sweep gas is typically a slip stream from the purified product, although other gases are occasionally used. When the product gas is used as sweep gas, very high-purity product gas can be obtained, but the recovery of the product gas is typically less than 95%.

Typical industrial flowsheets for PSA use 4 to 12 adsorbent vessels. With multiple vessels, the designer can sequence the switching valves to compensate for heating and cooling effects due to heat of adsorption and desorption, and also to economize on losses of product gas during depressurization, regeneration, and repressurization. Examples of typical commercial configurations are given by Ruthven et al. (1993), Cassidy and Doshi (1984), and Kumar et al. (1994).

Pressure swing adsorption is used in many processes; for example, air separation, hydrogen manufacture by steam reforming, and dehydration of ethanol–water azeotropic mixtures (see Section 17.6.5).

Temperature swing adsorption

Regeneration of the adsorbent by raising temperature is known as temperature swing adsorption (TSA). In TSA processes, heat is required to raise the temperature of the adsorbent, the vessel and piping, and to provide the heat of desorption. This heat is usually provided by flowing a hot stripping gas over the adsorbent. The stripping gas is typically steam, dry air, nitrogen, or a slip stream of purified product. The stripping gas must be chosen carefully to ensure that flammable atmospheres are not formed and the adsorbent is not deactivated. The stripping gas is usually heated in a fired heater, but electric or steam heaters are used in smaller plants.

After desorption is completed, the bed is usually flushed with cold purified product to bring the temperature back down to the adsorption temperature. Temperature swing processes typically operate on longer time cycles than PSA, as the cycle time is usually governed by the maximum attainable rates of heating and cooling.

Temperature swing adsorption is widely used for drying air and for removing trace amounts of organic compounds from vent gases using activated carbon as adsorbent. The activated carbon can then be regenerated with steam.

Adsorbent selection

Adsorbents for a reversible process such as PSA or TSA are chosen to give a wide range of adsorbent loading over an acceptable range of either temperature or pressure. Many adsorbents are proprietary materials that have been designed to have high specific surface area and hence give high loadings; however, isotherm data for common adsorbents such as activated carbon, alumina, silica gel, and some of the more common zeolites are available in the open literature and in books such as Breck (1974), Ruthven (1984), and Yang (2003).

Care must be taken to ensure that the adsorbent is not irreversibly poisoned by any component of the gas phase. When multiple contaminants must be removed from a gas, several layers of different adsorbents with selectivity for different contaminants can be loaded in the same vessel so that each contaminant is removed in turn.

Prices for some of the more common adsorbents are listed in Aspen ICARUS and other costing programs. Current prices for commodity adsorbents such as activated carbon, silica gel, and alumina can be found online or by contacting manufacturers.

Adsorption equipment design

Adsorption plants are often purchased from an industrial gas company as packaged modular plants that include the adsorbent, vessels, and valve skid. For TSA plants, the heater may also be included in the packaged plant scope. The design and optimization of PSA and TSA processes require detailed understanding of the adsorbent properties and heat of adsorption effects and are best left to specialist suppliers. The simplified method that follows is suitable for undergraduate design projects and for generating preliminary estimates.

When a plant is designed from scratch, the first step is to estimate the amount of adsorbent required. The amount of adsorbent can be determined from the flow rate of the adsorbed species and the change in the bed loading during the cycle. A mass balance on the bed gives:

$$(F_1 y_1 - F_2 y_2) M_w t_a = 1000 (m_1 - m_2) M_a f_L \tag{16.2}$$

where F_1 = feed molar flow rate (mol/s)
F_2 = product molar flow rate (mol/s)
y_1 = feed mole fraction of adsorbed component
y_2 = product mole fraction of adsorbed component

M_w = molecular weight of adsorbed component (g/mol)
t_a = time the bed is in the adsorption stage of the cycle (s)
m_1 = maximum adsorbent loading (g/g adsorbent)
m_2 = minimum adsorbent loading (g/g adsorbent)
M_a = mass of adsorbent per bed (kg)
f_L = fraction of bed that is fully loaded at end of adsorption phase of cycle

The fraction of the adsorbent bed, f_L, that reaches loading m_1 at the end of the adsorption step of the cycle depends on the process arrangement and the number of beds used. For a simple two-bed system it will usually be less than 0.7 unless a very sharp front is formed or a lead−lag arrangement can be used. With four or more beds, the cycle can usually be designed to give fractional loading close to 1.0 unless multiple components are being removed.

The time that the bed spends in the adsorption phase of the cycle is less than the total cycle time, which also includes time for regeneration, depressurizing, heating, cooling, etc. The rates of these processes are governed by intrinsic rates of desorption, mass transfer, and heat transfer. The development of rate-based models of these processes is discussed by Ruthven (1984) and Chhabra and Gurappa (2019). For a preliminary analysis, a time in the range of 5 to 60 minutes can be assumed for PSA and 60 to 200 minutes for TSA. The total cycle time is equal to the time spent in adsorption multiplied by the number of beds in the sequence.

The volume of each adsorbent bed can be estimated from the mass of adsorbent and the adsorbent bulk density. Fixed beds of adsorbent are usually used to give a sharp adsorption concentration profile. The adsorption vessel can then be sized as a cylindrical pressure vessel that contains the adsorbent volume, using the pressure vessel design methods given in Chapter 14. The head space is usually left empty, and up to 20% of the volume between the tangent lines of the vessel is packed with inert material to ensure that a uniform flow profile is established at the entry and exit of the bed and to prevent "fingering" of contaminant through the bed (Fig. 16.5). The aspect ratio of the bed is usually at least 3:1 to ensure that high fractional loading is obtained and the adsorbent is used efficiently.

The total plant cost will include at least two adsorbent vessels, the set of switching valves and any other equipment; such as blowers, vacuum pumps or heaters, that is required for regeneration.

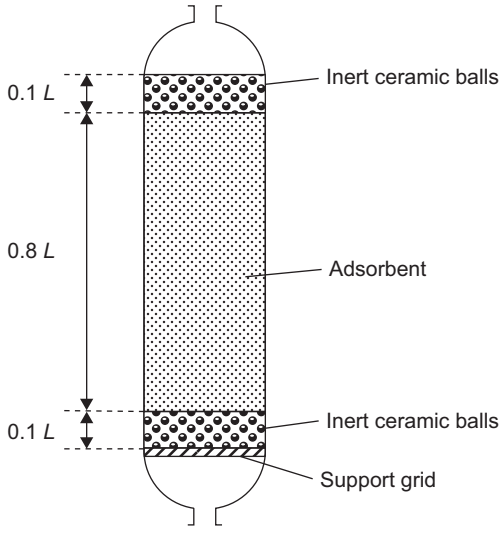


FIG. 16.5 Adsorption vessel internals.

Example 16.1

Yang et al. (1997) give isotherm data for adsorption of methane on zeolite 5A in the presence of hydrogen:

Pressure (atm)	0	1.5	2.5	4.5	6.5	9	12.5	16.5	19.5
Adsorbed amount (mmol/g)	0.0	0.4	0.7	1.0	1.25	1.45	1.6	1.7	1.75

It has been determined that a four-bed PSA plant using this adsorbent can be used to purify a stream containing 40% CH_4 in H_2 to give 90% recovery of hydrogen at purity 99.99 mol%. The adsorption time is 300s, and the beds are 85% loaded at the end of the adsorption step. If the feed gas is available at 25 atm and the off-gas can be discharged at 2 atm, estimate the amount of adsorbent per bed and the dimensions of each adsorbent vessel for a feed rate of 1000 kmol/h.

Data (Yang et al., 1997): Adsorbent bulk density = 795 kg/m^3.

Solution

Feed flow rate = 1000 kmol/h

hydrogen in feed = $1000 \times 0.60 = 600$ kmol/h

methane in feed = $1000 \times 0.40 = 400$ kmol/h, $y_{CH4,feed} = 0.4$

90% recovery at 99.99% purity:

hydrogen in product gas $= 600 \times 0.9 = 540$ kmol/h

methane in product gas $= \dfrac{(1-0.9999)}{0.9999} \times 540 = 5.4 \times 10^{-2}$ kmol/h

hydrogen in off–gas = $600 - 540 = 60$ kmol/h

methane in off–gas ≈ 400 kmol/h

So, methane mole fraction in off-gas, $y_{CH4,\ \text{off-gas}} = \dfrac{400}{460} = 0.870$

Partial pressures of methane:

in feed at 25 atm $= 25 \times 0.4 = 10$ atm

in off–gas at 2 atm = $2 \times 0.87 = 1.74$ atm

By fitting an isotherm through the data, plotting or interpolating, we find:

At 10 atm, adsorbent loading = 1.5 mmol/g

At 1.74 atm, adsorbent loading = 0.5 mmol/g

Substituting into Equation 16.2 (noting that we do not need the molecular weight, as the adsorbent loadings were given in mmol/g = mol/kg):

$$\{(1000 \times 0.4) - (540 \times 0.0001)\} \times \frac{1000}{3600} \times 300 = (1.5 - 0.5) \times M_a \times 0.85\ (\text{mol/s})$$

Hence, mass of adsorbent $M_a = \dfrac{400 \times 300}{3.6 \times 0.85 \times 1.0} = \underline{\underline{39,200\ \text{kg.}}}$

Volume of adsorbent bed $= \dfrac{39200}{795} = 49$ m^3.

Allow 20% of total volume for inert packing for good flow distribution, so tangent-to-tangent volume $= 49/0.8 = 61.7$ m^3.

Assume 4:1 cylinder, volume $= \dfrac{\pi\ D_T^2\ L_v}{4} = \pi {D_T}^3$

where D_T = vessel diameter

L_v = tangent-to-tangent length

So, ${D_T}^3 = 61.7/\pi$, vessel diameter = 2.70 m

Round up to nearest standard head size (see Chapter 14):

diameter = 2.74 m (9 ft)

tangent length = 11.0 m (36 ft)

We now have sufficient information to complete the pressure vessel design and costing (see Chapters 7 and 14). Note that four vessels will be needed and the total quantity of adsorbent is $4 \times 39{,}200$ kg = 156.8 t.

16.2.2 Membrane separation

A membrane is a thin layer of material that allows species to pass through by permeation. The material that flows through the membrane is known as the *permeate* and the material that does not is called the retentate. If some species

pass though the membrane faster than others, these species will accumulate in the permeate, and the membrane can be used to separate these components from the gas mixture.

The flux through a membrane is defined as the flow rate through a unit area of membrane per unit time. The flux is proportional to the applied partial pressure gradient:

$$M_i = \frac{P_i}{\delta}\left(p_{i,f} - p_{i,p}\right) \tag{16.3}$$

where M_i = molar flux of component i (mol/m^2.s)
P_i = permeability of membrane for component i (mol/m.s.bar)
δ = membrane thickness (m)
$p_{i,f}$ = local partial pressure of component i on feed side (bar)
$p_{i,p}$ = local partial pressure of component i on permeate side (bar)

The average flux across a long cylindrical membrane is given by:

$$M_{i,ave} = \frac{\int_0^{L_m} M_i \, dx}{L_m} \tag{16.4}$$

where $M_{i,ave}$ = average molar flux of component i (mol/m^2.s)
L_m = length of membrane (m)
x = length (m)

If the feed or permeate partial pressure varies substantially along the membrane length, an expression for the variation of partial pressure with length must be substituted into Equation 16.4 before the average flux can be found.

The ratio of permeability of two components is called the membrane selectivity, or ideal separation factor:

$$S_{ij} = \frac{P_i}{P_j} \tag{16.5}$$

where S_{ij} = selectivity of the membrane for component i over component j.

If the selectivity of the membrane for a component is very high, then that component can be recovered at high purity in the permeate.

At the retentate end of the membrane, the partial pressure of the permeating component is reduced; consequently, the driving force for permeation is lower and the flux is lower. If the partial pressure for the permeating species becomes too low, the flux becomes very low and an uneconomically large membrane area is required. Because of this effect, membrane processes for gas separation usually cannot achieve high purity in the retentate or high recovery of permeate. Techniques for maintaining an adequate flux at the retentate end are discussed later.

Membrane selection and construction

Membranes are described as *microporous* if they have an open pore structure and *dense* if there are no holes or pores. Microporous membranes perform essentially like sieves and allow small molecules to move through the pores while large molecules are blocked. The separation of $^{235}UF_6$ from $^{238}UF_6$ in uranium enrichment is the only commercial gas separation process that uses a microporous membrane. Most gas separations use *asymmetric* membranes, consisting of a very thin dense layer supported on a thick, porous layer that gives strength to the membrane (Fig. 16.6).

Gas separation membranes are usually made from elastomeric or glassy polymers, although very thin layers of metal or ceramic materials are used in some special applications. The use of polymers restricts membrane processes

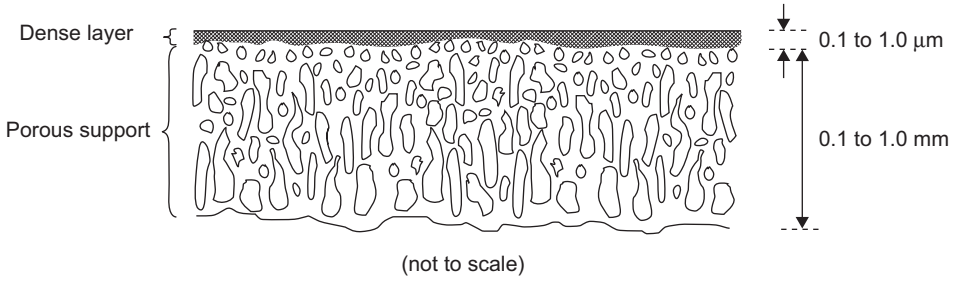


FIG. 16.6 Asymmetric membrane structure.

to operating at low temperatures; typically below 100 °C. For a dense membrane, the mechanism of permeation is for the gas to dissolve in the membrane on the feed side and then evaporate from the membrane on the permeate side. The membrane permeability and selectivity therefore depend on the solubility of different species in the membrane. With careful design and selection of membrane material, high selectivities can be obtained.

In addition to high selectivity, it is desirable to have high membrane permeability, as this will determine the area required, and hence the membrane cost. Table 16.1 gives permeability coefficients for some membrane materials. Other important parameters in membrane selection include mechanical stability, chemical resistance, thermal stability, ease of manufacture, and cost.

Gas separation membranes are usually manufactured as hollow fibers or else cast as flat sheets that are then spiral-wound into modular assemblies. Details of the manufacturing methods are given by Rautenbach and Albrecht (1989) and Scott and Hughes (1996). Hollow-fiber membranes are glued ("potted") into a resin to form a closure similar to the tube sheet of a shell and tube exchanger (Fig. 16.7). In a spiral-wound membrane, two membrane sheets are placed back to back and sealed along three edges to form an envelope. The fourth edge is attached to a perforated tube, from which the permeate can be withdrawn. Several membrane envelopes can be

TABLE 16.1 Membrane permeability coefficients [cm^3(STP).cm/cm^2.s.cmHg] $\times 10^{10}$

Membrane	Temperature (°C)	CO_2	O_2	N_2
Natural rubber	25	99.6	17.7	6.12
Ethyl cellulose	25	113	15	3.0
Polystyrene	20	10.0	2.01	0.32
Polycarbonate	25	8.0	1.4	0.3
Poly(dimethylsiloxane)	25	3240	605	300
Poly(ethylene phthalate)	25	0.15	0.03	0.006
Poly(vinyl alcohol)	20	0.0005	0.00052	0.00045

From Osada and Nakagawa, 1992.

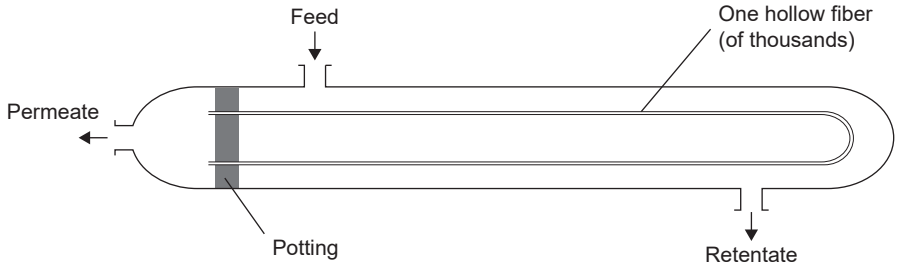


FIG. 16.7 Hollow-fiber membrane module.

attached to one tube, with netlike spacers between them. The entire assembly is then wrapped into a spiral and inserted into a tubular shell with a suitable head assembly through which the permeate can be withdrawn (Fig. 16.8).

Both the hollow-fiber and spiral-wound designs use dead-ended membranes that do not allow the use of a sweep gas on the permeate side. The permeate stream can be withdrawn from the feed end or retentate end, giving countercurrent or co-current flow (Fig. 16.9). With spiral-wound membranes, the permeate stream can also be withdrawn from both ends, giving an approximation of cross flow (see Fig. 16.9c). The choice of flow arrangement determines the boundary conditions for integrating Equation 16.4; see Chapter 5 of Scott and Hughes (1996).

In both the hollow-fiber and spiral-wound designs, the cost of the membrane itself is typically 80% to 90% of the total module cost.

Membrane process design

A typical membrane process uses a large number of membrane modules to achieve the overall separation. The modules can be arranged in various networks, depending on the processing objective and membrane performance. Some of the more common arrangements are illustrated in Fig. 16.10 and described here.

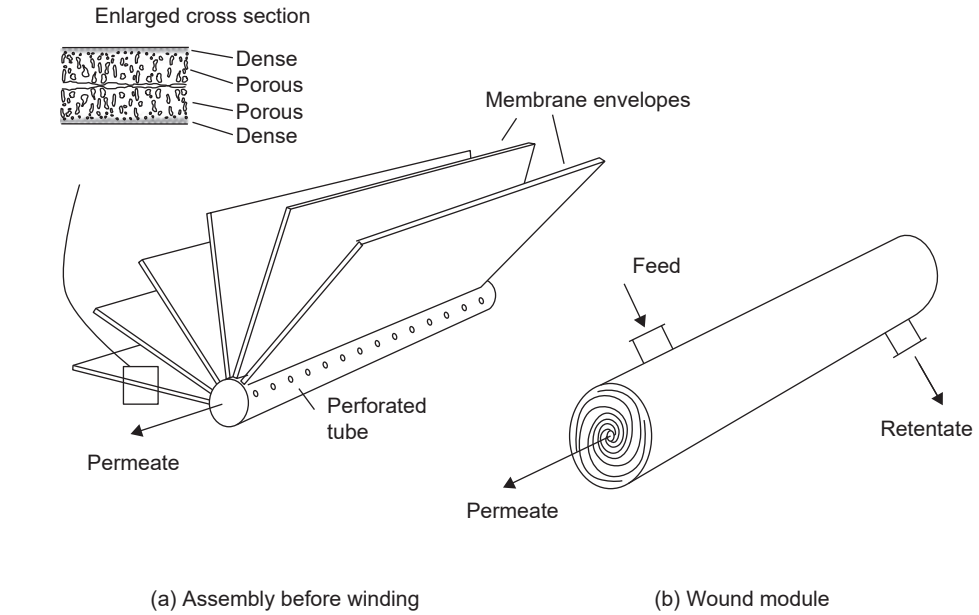


FIG. 16.8 Spiral-wound membrane module.

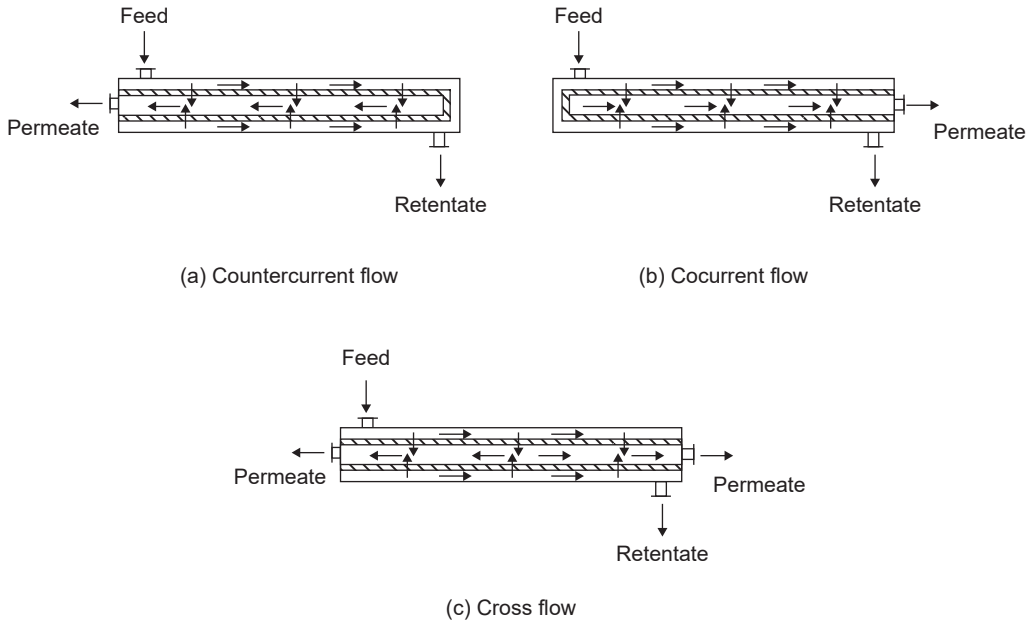


FIG. 16.9 Membrane flow patterns.

1. Tapered cascade (see Fig. 16.10a). This flow scheme is used when the final retentate flow is a small fraction of the feed flow rate. It ensures that the retentate side velocities are maintained in downstream modules as the flow rate decreases. Tapered cascades with retentate or permeate recycle can also be used.
2. Permeate recycle (see Fig. 16.10b). The use of a permeate recycle increases both the recovery and the purity of the permeate. The permeate stream from the downstream module is recycled to the feed of the upstream module. This increases the concentration and partial pressure of the permeating species in the first module, leading to better permeate purity and higher flux. The downstream module can be run to higher recovery, even if this causes the purity obtained in the downstream module to be lower.

3. Retentate recycle (see Fig. 16.10c). In this scheme, the permeate stream from a first module is sent to a second module. Retentate from the second module is recycled to the first module. This flow scheme is used to increase permeate purity when the membrane average selectivity is low. In some cases, several modules can be placed in series, with retentate recycle from the downstream module to the preceding module.

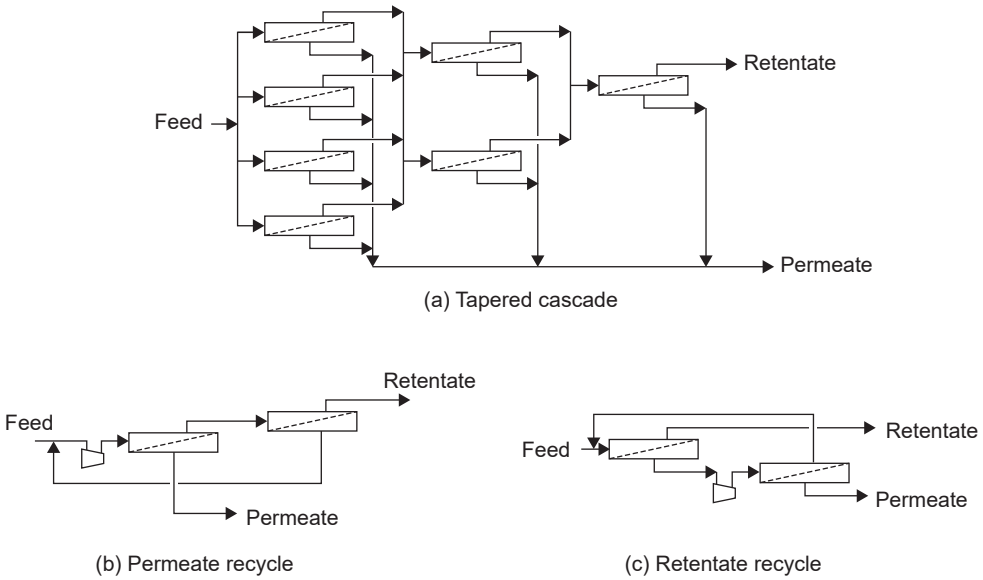


FIG. 16.10 Membrane flow schemes.

In addition to the membrane modules, membrane separation units often incorporate chillers, condensers, heaters, and guard beds. If the feed contains condensable components, these are usually knocked out by chilling and condensing upstream of the membrane so that they do not condense on the membrane and "blind" the surface. The gas is then reheated to give a comfortable margin of temperature above the dew point. When a network of membrane modules is used, intermediate chillers, condensers, and reheaters may be needed if the condensable components build up to the dew point concentration in either the permeate or the retentate of an intermediate module. Recompression between stages may also be necessary, but is avoided whenever possible, because of the expense of compression.

Sometimes, condensable or reactive species can poison or permanently damage the membrane. In such cases, these components are removed upstream of the membrane unit, usually by using an adsorption process.

The design of membrane separation plants is usually left to specialist vendors. Details of the membrane design and construction are usually proprietary, and optimal process design requires careful selection of flow pattern, flow scheme, and ancillary equipment. Accurate prediction of the overall purity and recovery requires a good knowledge of the permeability of all species present so that Equation 16.4 can be integrated for every species simultaneously. Design methods for membrane units are described in Scott and Hughes (1996), Noble and Stern (1995), Mulder (1996), Hoffman (2003), Sridhar and Moulik (2018), and Baker (2012). Short-cut design methods are given by Hogsett and Mazur (1983) and Fleming and Dupuis (1993), but both papers caution that final design should be left to experts. A simplified membrane design example is given in Example 16.6 in Section 16.5.4 for the purification of water by reverse osmosis. Gas separations are more complex in that there are usually multiple species that permeate through the membrane.

The proprietary nature of membrane technology for gas separations means that there is little reliable cost information in the open literature. The *Handbook of Gas Processing Processes* published biennially as a supplement to *Hydrocarbon Processing* usually provides some information from vendors that can be used to make preliminary estimates.

16.2.3 Cryogenic distillation

In cryogenic distillation, the feed gas is compressed to high pressure, cooled, and then chilled until the gas is partially liquefied and distillation can be carried out. The refrigeration load for chilling the gas may be met by expansion of the products or by using an external refrigeration cycle. The distillation column is designed to operate at very low temperatures and usually has many stages, but other than that is much like any conventional distillation; see Chapter 17.

The efficiency of cryogenic separations depends critically on heat recovery (cold recovery) during chilling of the feed. Very close temperature approaches of the order of 1 to 5 °C are used to minimize the amount of low-temperature refrigeration that is needed. Complex multilevel refrigeration cycles are also used to improve the coefficient of performance and reduce the compression work. The design of refrigeration cycles and heat recovery networks is covered in Chapter 3.

If the pressure of a cryogenic process is increased, the process can be carried out closer to ambient temperature, giving a smaller temperature range for the refrigeration cycle and hence a more efficient refrigeration (see Section 3.2.6). It also becomes easier to generate the required refrigeration by expansion of the products; however, the feed compression becomes more costly and the distillation becomes more difficult, as relative volatility generally decreases with increased pressure. One of the main trade-offs in design of cryogenic processes is therefore between feed compression and refrigeration plant compression.

Cryogenic distillation is usually the lowest-cost process when handling large quantities of gases heavier than hydrogen. It is widely used industrially for air separation, natural gas liquids recovery, ethylene recovery, and propylene recovery; see Flynn (2004).

16.2.4 Absorption and stripping

In an absorption process, a component is removed from a gas by contacting the gas with a solvent that dissolves the component selectively. The solvent is then regenerated in a stripping process and recycled to the absorber.

Absorption can take place through physical dissolution of gas components in the liquid phase (*physisorption*) or chemical reaction between gas-phase components and the liquid phase (*chemisorption*). Absorption can be very cost-effective if a solvent can be found that has high affinity for the desired gas-phase components. Absorption is widely used for the removal of acid gases such as carbon dioxide, hydrogen sulfide, and sulfur dioxide, using basic solutions as solvent.

Absorption and stripping are usually carried out in vapor–liquid contacting columns; see Section 17.14.

16.2.5 Condensation

A condensable vapor can be recovered from a mixture with other gases that have much lower dew points by simple condensation. Any type of heat exchanger can be used as a condenser, although conventional shell and tube exchangers are most common. When one component is condensed from a non-condensing gas, the process is known as partial condensation, and care must be taken to include mass transfer limitations, as well as heat transfer in the exchanger design. The design of partial condensers is covered as a part of the treatment of heat exchanger design in Section 19.10.8.

When a partial condenser is used, it will often be followed by a settling drum to ensure that condensed liquid is not entrained into the gas flow. The design of vapor–liquid settling drums is discussed in Section 16.3.

The extent of recovery that can be accomplished by condensation depends on the temperature, pressure, and phase equilibrium properties of the mixture. The process performance is easily predicted using equilibrium flash models in commercial process simulation programs, as described in Chapter 4.

Recovery of the condensed component can be increased by operating at higher pressure or lower temperature. In situations where the initial concentration of condensed component is high, it may be economical to use two or more stages of condensation, with the later stages operated at lower temperature or higher pressure. This obviates cooling all of the condensed liquid to the lowest temperature or compressing the entire vapor to the highest pressure.

16.3 Gas–liquid separators

The separation of entrained liquid droplets and mists from gas or vapor streams is possible whenever the temperature of a vapor is lowered below the dew point. Where the carryover of some fine droplets can be tolerated, it is often sufficient to rely on gravity settling in a vertical or horizontal separating vessel (known as a knockout pot). Knockout pots are often used immediately downstream of condensers or coolers to prevent entrainment of liquid and two-phase flow in downstream vapor lines. Knockout pots are also used before compressors and between intermediate stages of compressors to prevent liquid droplets from damaging the compressor blades.

Knitted mesh demisting pads are frequently used to improve the performance of separating vessels where the droplets are likely to be small, down to 1 μm, and where high separating efficiencies are required. Proprietary demister pads are available in a wide range of materials, metals and plastics; thickness and pad densities. For liquid separators, stainless steel pads around 100 mm thick and with a nominal density of 150 kg/m^3 would generally be used. Use of a demister pad allows a smaller vessel to be used. Separating efficiencies above 99% can be obtained with low-pressure drop. The design and specification of demister pads for gas–liquid separators are discussed by Pryce Bailey and Davies (1973. The design methods for horizontal separators given later are based on a procedure given by Gerunda (1981).

The separation of liquid droplets and mists from gas or vapor streams is analogous to the separation of solid particles from gas flows, and with the possible exception of filtration, the same techniques and equipment can be used; see Section 18.5. Cyclone separators are frequently used for gas–liquid separation. They can be designed using the same methods used for gas–solids cyclones. The inlet velocity should be kept below 30 m/s to avoid pick-up of liquid from the cyclone surfaces.

16.3.1 Settling velocity

Equation 16.6 can be used to estimate the settling velocity of the liquid droplets for the design of separating vessels.

$$u_t = 0.07[(\rho_L - \rho_v)/\rho_v]^{1/2} \tag{16.6}$$

where u_t = settling velocity, m/s
ρ_L = liquid density, kg/m^3
ρ_v = vapor density, kg/m^3

If a demister pad is not used, the value of u_t obtained from Equation 16.6 should be multiplied by a factor of 0.15 to provide a margin of safety and to allow for flow surges.

16.3.2 Vertical separators

The layout and typical proportions of a vertical gas–liquid separator are shown in Fig. 16.11.

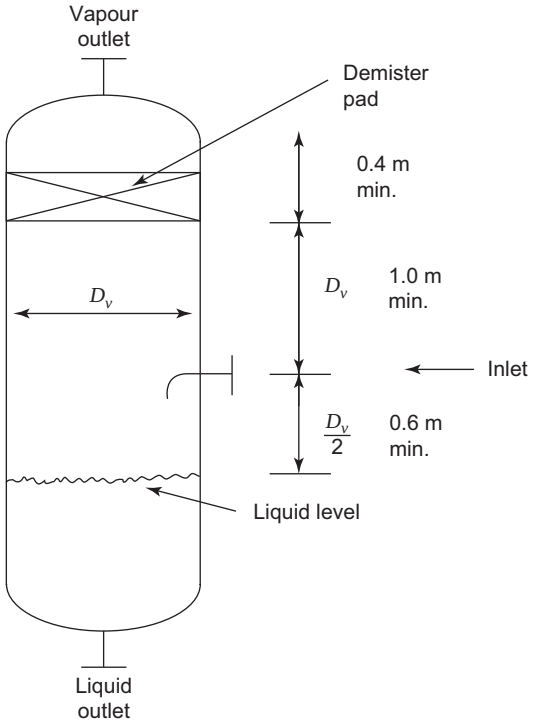


FIG. 16.11 Vertical liquid–vapor separator.

The diameter of the vessel must be large enough to slow the gas down to below the velocity at which the droplets will settle out. So the minimum allowable diameter will be given by:

$$D_v = \sqrt{\left(\frac{4V_v}{\pi u_s}\right)} \tag{16.7}$$

where Dv = minimum vessel diameter, m
Vv = gas or vapor volumetric flow rate, m^3/s
$u_s = u_t$ if a demister pad is used, and 0.15 u_t for a separator without a demister pad; u_t from Equation 16.6, m/s

The diameter is usually rounded up to the nearest standard vessel size so that standard vessel closures can be used; see Section 14.5.2.

The height of the vessel outlet above the gas inlet should be sufficient to allow for disengagement of the liquid drops. A height equal to the diameter of the vessel or 1 m, whichever is the greatest, should be used (see Fig. 16.11).

The liquid level will depend on the hold-up time necessary for smooth operation and control; typically 10 minutes of liquid hold-up would be allowed.

Example 16.2

Make a preliminary design for a separator to separate a mixture of steam and water; flow rates: steam 2000 kg/h, water 1000 kg/h; operating pressure 4 bar.

Solution

From steam tables, at 4 bar: saturation temperature 143.6 °C, liquid density 926.4 kg/m^3, and vapor density 2.16 kg/m^3.

$$u_t = 0.07[(926.4 - 2.16)/2.16]^{\frac{1}{2}} = 1.45 \text{ m/s} \tag{16.6}$$

As the separation of condensate from steam is unlikely to be critical, a demister pad will not be specified.

$$\text{So, } u_t = 0.15 \times 1.45 = 0.218 \text{ m/s}$$

$$\text{Vapor volumetric flow rate} = \frac{2000}{3600 \times 2.16} = 0.257 \text{ m}^3/\text{s}$$

$$D_v = \sqrt{[(4 \times 0.257)/(\pi \times 0.218)]} = 1.23 \text{ m, round to nearest standard vessel size, 1.25 m (4 ft)} \tag{16.7}$$

$$\text{Liquid volumetric flow-rate} = \frac{1000}{3600 \times 926.14} = 3.0 \times 10^{-4} \text{ m}^3/\text{s}$$

Allow a minimum of 10 minutes hold-up.

$$\text{Volume held in vessel} = 3.0 \times 10^{-4} \times (10 \times 60) = 0.18 \text{ m}^3$$

$$\text{Liquid depth required, } h_L = \frac{\text{volume held up}}{\text{vessel cross sectional area}}$$

$$= \frac{0.18}{(\pi \times 1.25^2/4)} = 0.15 \text{ m}$$

Increase to 0.3 m to allow space for positioning the level controller.

16.3.3 Horizontal separators

The layout of a typical horizontal separator is shown in Fig. 16.12. A horizontal separator would be selected when a longer liquid hold-up time is required, for example, to give better process control of the liquid flow.

In the design of a horizontal separator, the vessel diameter cannot be determined independently of its length, unlike for a vertical separator. The diameter and length, and the liquid level, must be chosen to give sufficient vapor residence time for the liquid droplets to settle out and for the required liquid hold-up time to be met.

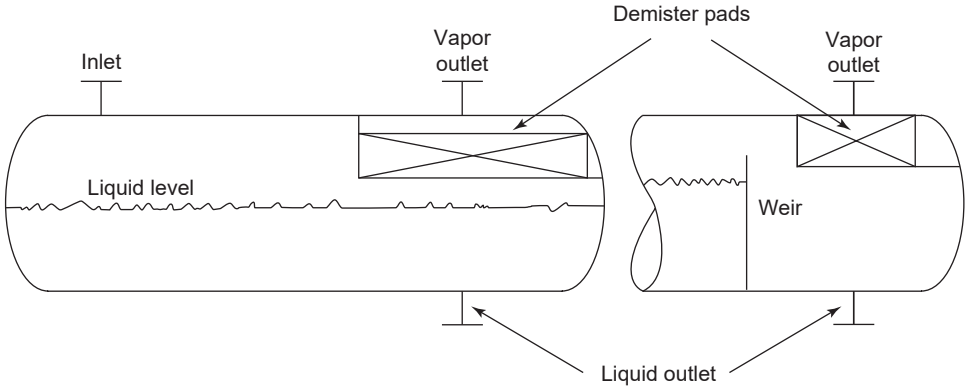


FIG. 16.12 Horizontal liquid–vapor separator.

The most economical length-to-diameter ratio will depend on the operating pressure (see Chapter 14). As a general guide, the following values can be used:

Operating pressure, bar	Length/diameter, L_v/D_v
0–20	3
20–35	4
>35	5

The relationship between the area for vapor flow, A_v, and the height above the liquid level, h_v, can been found from tables giving the dimensions of the segments of circles; see Green and Southard (2018) or Figs. 17.39 and 17.40 in Chapter 17.

For preliminary designs, set the liquid height at half the vessel diameter,

$$h_v = D_v/2 \text{ and } f_v = 0.5$$

where f_v is the fraction of the total cross-sectional area occupied by the vapor.

The design procedure for horizontal separators is illustrated in the following example.

Example 16.3

Design a horizontal separator to separate 10,000 kg/h of liquid, density 962.0 kg/m^3, from 12,500 kg/h of vapor, density 23.6 kg/m^3. The vessel operating pressure will be 21 bar.

Solution

$$u_t = 0.07[(962.0 - 23.6)/23.6]^{1/2} = 0.44 \text{ m/s}$$

Try a separator without a demister pad.

$$u_s = 0.15 \times 0.44 = 0.066 \text{ m/s}$$

$$\text{Vapor volumetric flow rate} = \frac{12{,}500}{3600 \times 23.6} = 0.147 \text{ m}^3/\text{s}$$

Take $h_v = 0.5D_v$ and $L_v/D_v = 4$

$$\text{Cross-sectional area for vapor flow} = \frac{\pi D_v^2}{4} \times 0.5 = 0.393\, D_v^2$$

$$\text{Vapor velocity, } u_v = \frac{0.147}{0.393 D_v^2} = 0.374\, D_v^{-2}$$

Vapor residence time required for the droplets to settle to liquid surface:

$$h_v / u_s = 0.5D_v/0.066 = 7.58D_v$$

Actual residence time = vessel length/vapor velocity:

$$= \frac{L_v}{u_v} = \frac{4D_v}{0.374D_v^{-2}} = 10.70D_v^3$$

For satisfactory separation, required residence time = actual:

$$\text{So, } 7.58D_v = 10.70D_v^3$$

$$D_v = 0.84 \text{ m, say } 0.92 \text{ m (3 ft, standard pipe size)}$$

Liquid hold-up time:

$$\text{liquid volumetric flow} - \text{rate} = \frac{10{,}000}{3600 \times 962.0} = 0.00289 \text{ m}^3/\text{s}$$

$$\text{liquid cross}-\text{sectional area} = \frac{\pi \times 0.92^2}{4} \times 0.5 = 0.332 \text{ m}^2$$

$$\text{Length}, L_v = 4 \times 0.92 = 3.7 \text{ m}$$

$$\text{Hold}-\text{up volume} = 0.332 \times 3.7 = 1.23 \text{ m}^3$$

$$\text{Hold}-\text{up time} = \text{liquid volume/liquid flow rate}$$

$$= 1.23/0.00289 = 426 \text{ s} = 7 \text{ minutes}$$

This is unsatisfactory, 10 minutes minimum required.

Need to increase the liquid volume. This is best done by increasing the vessel diameter. If the liquid height is kept at half the vessel diameter, the diameter must be increased by a factor of roughly (10/7)0.5 = 1.2.

$$\text{New } D_v = 0.92 \times 1.2 = 1.1 \text{ m}$$

Check liquid residence time:

$$\text{new liquid volume} = \frac{\pi \times 1.1^2}{4} \times 0.5 \times (4 \times 1.1) = 2.09 \text{ m}^3$$

$$\text{new residence time} = 2.09/0.00289 = 723 \text{ s} = 12 \text{ minutes, satisfactory}$$

Increasing the vessel diameter will have also changed the vapor velocity and the height above the liquid surface. The liquid separation will still be satisfactory, as the velocity, and hence the residence time, is inversely proportional to the diameter squared, whereas the distance the droplets have to fall is directly proportional to the diameter.

In practice, the distance traveled by the vapor will be less than the vessel length, L_v, as the vapor inlet and outlet nozzles will be set in from the ends. This could be allowed for in the design but will make little difference.

16.4 Liquid–liquid separation

Separation of two liquid phases, immiscible or partially miscible liquids, is a common requirement in the process industries. For example, in single-stage liquid–liquid extraction, the liquid-contacting step must be followed by a settling stage. It is also frequently necessary to separate small quantities of entrained water from organic-phase process streams. The simplest form of equipment used to separate liquid phases is the gravity settling tank, the decanter. Various types of proprietary equipment are also used to promote coalescence and improve separation in difficult systems or where emulsions are likely to form. Centrifuges and hydrocyclones are also used.

Liquid–liquid extraction can also be carried out as a multistage countercurrent process. This is described with other multistage separation processes in Chapter 17, Section 17.16.

16.4.1 Decanters (settlers)

Decanters are used to separate liquids where there is a sufficient difference in density between the liquids for the droplets to settle readily. Decanters are essentially tanks that give sufficient residence time for the droplets of the dispersed phase to rise (or settle) to the interface between the phases and coalesce. In an operating decanter there will be three distinct zones or bands: clear heavy liquid; separating dispersed liquid (the dispersion zone); and clear light liquid.

Decanters are normally designed for continuous operation, but the same design principles apply to batch-operated units. Many vessel shapes are used for decanters, but for most applications a cylindrical vessel will be suitable and will be the cheapest shape. Typical designs are shown in Figs. 16.13 and 16.14. The position of the interface can be controlled, with or without the use of instruments, by use of a siphon take-off for the heavy liquid (see Fig. 16.13).

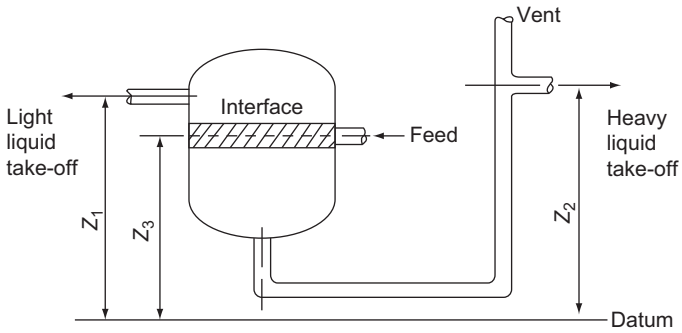


FIG. 16.13 Vertical decanter.

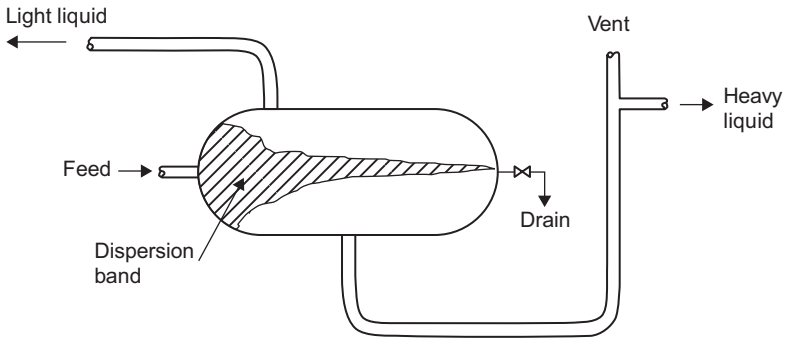


FIG. 16.14 Horizontal decanter.

The height of the take-off can be determined by making a pressure balance. Neglecting friction loss in the pipes, the pressure exerted by the combined height of the heavy and light liquid in the vessel must be balanced by the height of the heavy liquid in the take-off leg (see Fig. 16.13).

$$(z_1 - z_3)\rho_1 g + z_3\rho_2 g = z_2\rho_2 g$$

hence

$$z_2 = \frac{(z_1 - z_3)\rho_1}{\rho_2} + z_3 \tag{16.8}$$

where ρ_1 = density of the light liquid, kg/m^3
ρ_2 = density of the heavy liquid, kg/m^3
z_1 = height from datum to light liquid overflow, m
z_2 = height from datum to heavy liquid overflow, m
z_3 = height from datum to the interface, m

The height of the liquid interface should be measured accurately when the liquid densities are close, when one component is present only in small quantities, or when the throughput is very small. A typical scheme for the automatic control of the interface, using a level instrument that can detect the position of the interface, is shown

in Fig. 16.15. Where one phase is present only in small amounts, it is often recycled to the decanter feed to give more stable operation.

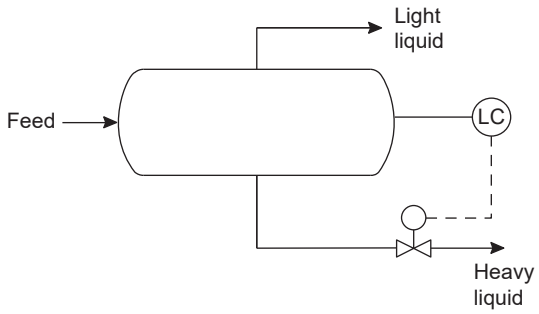


FIG. 16.15 Automatic control, level controller detecting interface.

Decanter design

A rough estimate of the decanter volume required can be made by taking a hold-up time of 5 to 10 minutes, which is usually sufficient where emulsions are not likely to form. Methods for the design of decanters are given by Hooper (1997) and Signales (1975). The general approach taken is outlined here and illustrated by Example 16.4.

The decanter vessel is sized on the basis that the velocity of the continuous phase must be less than the settling velocity of the droplets of the dispersed phase. Plug flow is assumed, and the velocity of the continuous phase is calculated using the area of the interface:

$$u_c = \frac{L_c}{A_i} < u_d \tag{16.9}$$

where u_d = settling velocity of the dispersed phase droplets, m/s,
u_c = velocity of the continuous phase, m/s
L_c = continuous-phase volumetric flow rate, m^3/s
A_i = area of the interface, m^2

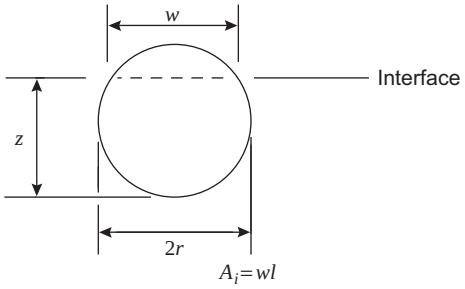
Stokes law is used to determine the settling velocity of the droplets:

$$u_d = \frac{d_d^2 g(\rho_d - \rho_c)}{18\mu_c} \tag{16.10}$$

where d_d = droplet diameter, m
u_d = settling (terminal) velocity of the dispersed-phase droplets with diameter d, m/s
ρ_c = density of the continuous phase, kg/m^3
ρ_d = density of the dispersed phase, kg/m^3
μ_c = viscosity of the continuous phase, $N\ s/m^2$
g = gravitational acceleration, 9.81 m/s^2

Equation 16.10 is used to calculate the settling velocity with an assumed droplet size of 150 μm, which is well below the droplet sizes normally found in decanter feeds. If the calculated settling velocity is greater than 4×10^{-3} m/s, then a figure of 4×10^{-3} m/s is used.

For a horizontal, cylindrical, decanter vessel, the interfacial area will depend on the position of the interface.



and

$$w = 2\left(2rs - z^2\right)^{1/2}$$

where w = width of the interface, m
z = height of the interface from the base of the vessel, m
l = length of the cylinder, m
r = radius of the cylinder, m

For a vertical, cylindrical decanter:

$$A_i = \pi r^2$$

The position of the interface should be such that the band of droplets that collect at the interface waiting to coalesce and cross the interface does not extend to the bottom (or top) of the vessel. Ryon et al. (1959) and Mizrahi and Barnea (1973) have shown that the depth of the dispersion band is a function of the liquid flow rate and the interfacial area. A value of 10% of the decanter height is usually taken for design purposes. If the performance of the decanter is likely to be critical to process performance, the design can be investigated using scale models. The model should be scaled to operate at the same Reynolds number as the proposed design so that the effect of turbulence can be investigated; see Hooper (1975).

Example 16.4

Design a decanter to separate a light oil from water. The oil is the dispersed phase.

Oil, flow rate 1000 kg/h, density 900 kg/m^3, viscosity 3 mN s/m^2
Water, flow rate 5000 kg/h, density 1000 kg/m^3, viscosity 1 mN s/m^2

Solution

Take $d_d = 150$ μm:

$$u_d = \frac{(150 \times 10^{-6})^2 9.81(900 - 1000)}{18 \times 1 \times 10^{-3}} \tag{16.10}$$

$$= -0.0012 \text{ m/s}, \ -1.2 \text{ mm/s (rising)}$$

Because the flow rate is small, use a vertical, cylindrical vessel.

$$L_c = \frac{5000}{1000} \times \frac{1}{3600} = 1.39 \times 10^{-3} \text{ m}^3/\text{s}$$

$$u_c \leq u_d, \text{ and } u_c = \frac{L_c}{A_i}$$

hence

$$A_i = \frac{1.39 \times 10^{-3}}{0.0012} = 1.16 \text{ m}^2$$

$$r = \sqrt{\frac{1.16}{\pi}} = 0.61 \text{ m}$$

$$\text{diameter} = \underline{\underline{1.2 \text{ m}}}$$

Take the height as twice the diameter, a reasonable value for a decanter:

$$\text{height} = \underline{\underline{2.4 \text{ m}}}$$

Take the dispersion band as 10% of the height = $\underline{\underline{0.24 \text{ m}}}$.
Check the residence time of the droplets in the dispersion band:

$$\frac{0.24}{u_d} = \frac{0.24}{0.0012} = 200 \text{ s } (\sim 3 \text{ min})$$

This is satisfactory, a time of 2 to 5 minutes is normally recommended for control purposes. Check the size of the water (continuous, heavy phase) droplets that could be entrained with the oil (light phase).

$$\text{Velocity of oil phase} = \frac{1000}{900} \times \frac{1}{3600} \times \frac{1}{1.16}$$

$$= 2.7 \times 10^{-4} \text{ m/s } (0.27 \text{ mm/s})$$

From Equation 16.10:

$$d_d = \left[\frac{u_d 18 \mu_c}{g(\rho_d - 2\rho_c)}\right]^{1/2}$$

so the entrained droplet size will be:

$$= \left[\frac{2.7 \times 10^{-4} \times 18 \times 3 \times 10^{-3}}{9.81(1000 - 900)}\right]^{1/2}$$

$$= 1.2 \times 10^{-4} \text{ m} = 120 \ \mu\text{m}$$

which is satisfactory; below 150 μm.

Piping arrangement

To minimize entrainment by the jet of liquid entering the vessel, the inlet velocity for a decanter should be kept below 1 m/s.

$$\text{Flow-rate} = \left[\frac{1000}{900} + \frac{5000}{1000}\right] \ \frac{1}{3600} = 1.7 \times 10^{-3} \text{ m}^3/\text{s}$$

$$\text{Area of pipe} = \frac{1.7 \times 10^{-3}}{1} = 1.7 \times 10^{-3} \text{ m}^2$$

$$\text{Pipe diameter} = \sqrt{\frac{1.7 \times 10^{-3} \times 4}{\pi}} = 0.047 \text{ m, say } \underline{\underline{50 \text{ mm}}}$$

Take the position of the interface as halfway up the vessel and the light liquid off-take as at 90% of the vessel height; then:

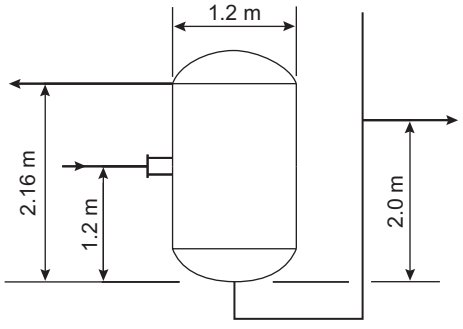
$$z_1 = 0.9 \times 2.4 = 2.16 \text{ m}$$

$$z_3 = 0.5 \times 2.4 = 1.2 \text{ m}$$

$$z_2 = \frac{(2.16 - 1.2)}{1000} \times 900 + 1.2 = \underline{\underline{2.06 \text{ m}}} \tag{16.8}$$

$$\text{say } \underline{\underline{2.0 \text{ m}}}$$

The proposed design:



Drain valves should be fitted at the interface so that any tendency for an emulsion to form can be checked and the emulsion accumulating at the interface drained off periodically as necessary.

16.4.2 Plate separators

Stacks of horizontal, parallel plates are used in some proprietary decanter designs to increase the interfacial area per unit volume and to reduce turbulence. They effectively convert the decanter volume into several smaller separators connected in parallel.

16.4.3 Coalescers

Proprietary equipment, in which the dispersion is forced through some form of coalescing medium, is often used for the coalescence and separation of finely dispersed droplets. A medium is chosen that is preferentially wetted by the dispersed phase; knitted wire or plastic mesh, beds of fibrous material, or special membranes are used. The coalescing medium works by holding up the dispersed droplets long enough for them to form globlets of sufficient size to settle. A typical unit is shown in Fig. 16.16; see Redmon (1963). Coalescing filters are suitable for separating small quantities of dispersed liquids from large throughputs.

Electrical coalescers, in which a high-voltage field is used to break down the stabilizing film surrounding the suspended droplets, are used for desalting crude oils and for similar applications; see Waterman (1965).

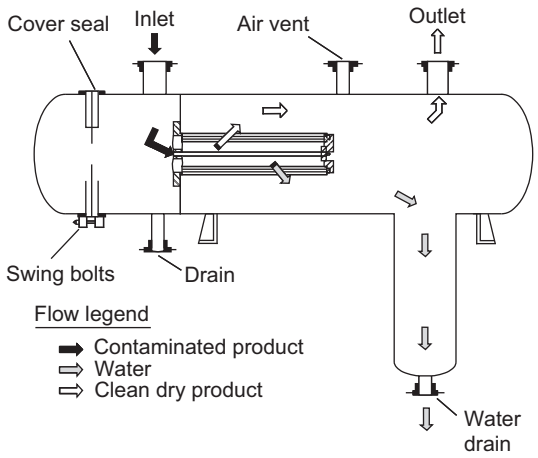


FIG. 16.16 Typical coalescer design.

16.4.4 Centrifugal separators

Liquid–liquid mixtures can be separated in the same centrifugal devices that are used for liquid–solid separations; see Section 18.6.

Sedimentation centrifuges

For difficult separations, where simple gravity settling is not satisfactory, sedimentation centrifuges should be considered. Centrifuging will give a cleaner separation than that obtainable by gravity settling. Centrifuges can be used where the difference in specific gravity between the liquids is very small, as low as 100 kg/m^3, and they can handle high throughputs, up to around 100 m^3/h. Also, centrifuging will usually break any emulsion that may form. Bowl or disc centrifuges are normally used (see Section 18.6.3).

Hydrocyclones

Hydrocyclones are used for some liquid–liquid separations, but are not as effective in this application as in separating solids from liquids, as the high shear in a hydrocyclone can cause re-entrainment of droplets. The design of hydrocyclones is discussed in Section 18.6.4.

16.5 Separation of dissolved components

Liquid-phase solutions are present in almost every chemical process. The most commonly used techniques for the separation and purification of miscible liquids are distillation and solvent extraction. In recent years, adsorption, ion exchange, and chromatography have become practical alternatives to distillation or solvent extraction in many special applications.

Gases that are dissolved in a liquid can be removed by stripping; see Section 16.2.4.

Distillation is probably the most widely used separation technique in the chemical process industries and is covered in Chapter 17 of this book. When a liquid mixture can be separated by distillation, this will usually be the most economical approach; however, distillation cannot be used for dissolved solids, salts, thermally sensitive compounds, or macromolecules that have low volatility. A large number of valuable product molecules, including many specialty chemicals and most active pharmaceutical ingredients and biochemicals, fall into these categories and require alternative separation processes.

Solvent extraction and the associated technique, leaching (solid−liquid extraction), are described later and in Section 17.16.

Components that will form a solid phase can be recovered from liquid solution by crystallization or precipitation. Crystallization and precipitation processes are usually followed by filtration, centrifugation, drying, and other solids-handling processes. The solids formation process usually controls particle size, shape, and strength, so the operations used to form and grow particles often dictate the requirements of the downstream equipment; see Chapter 18.

Ion exchange can be used to recover charged particles. Ion exchange is used to substitute one ion for another in electrolyte solutions; for example, replacing a metal cation with H^+ to form an acid that can then be recovered by distillation.

Membrane separations can be used for large molecules, for reverse osmosis, and for concentration of slurries. Membranes can also be used when a solvent- or solute-selective membrane material can be developed.

Adsorption can be used to selectively remove a dissolved liquid or solid component from solution. When the adsorbent is regenerated by elution with a solvent, the process is known as preparative chromatography (for small-production volumes) or *production chromatography* (for large volumes), which are discussed in Section 16.5.8. Adsorption with regeneration by cycling temperature or pressure is less commonly used for liquids.

16.5.1 Evaporators

On an industrial scale, evaporation and crystallization are the main processes used for the recovery of dissolved solids from solutions. Evaporation is the removal of a solvent by vaporization from solids that are not volatile. It is normally used to produce a concentrated liquid, often before crystallization, but a dry solid product can be obtained with some specialized designs. The general subject of evaporation is covered in Chhabra and Gurappa (2019). The selection of the appropriate type of evaporator is discussed by Cole (1984) and Gabelman (2020). Evaporation is the subject of a book by Billet (1989).

Many evaporator designs have been developed for specialized applications in particular industries. The designs can be grouped into the following basic types.

Direct-heated evaporators

This type includes solar pans and submerged combustion units. Submerged combustion evaporators can be used for applications where contamination of the solution by the products of combustion is acceptable.

Long-tube evaporators (Fig. 16.17)

In this type, the liquid flows as a thin film on the walls of a long, vertical, heated tube. Both falling film and rising film types are used. They are high-capacity units suitable for low-viscosity solutions.

Forced-circulation evaporators (Fig. 16.18)

In forced-circulation evaporators the liquid is pumped through the tubes. They are suitable for use with materials that tend to foul the heat transfer surfaces and where crystallization can occur in the evaporator.

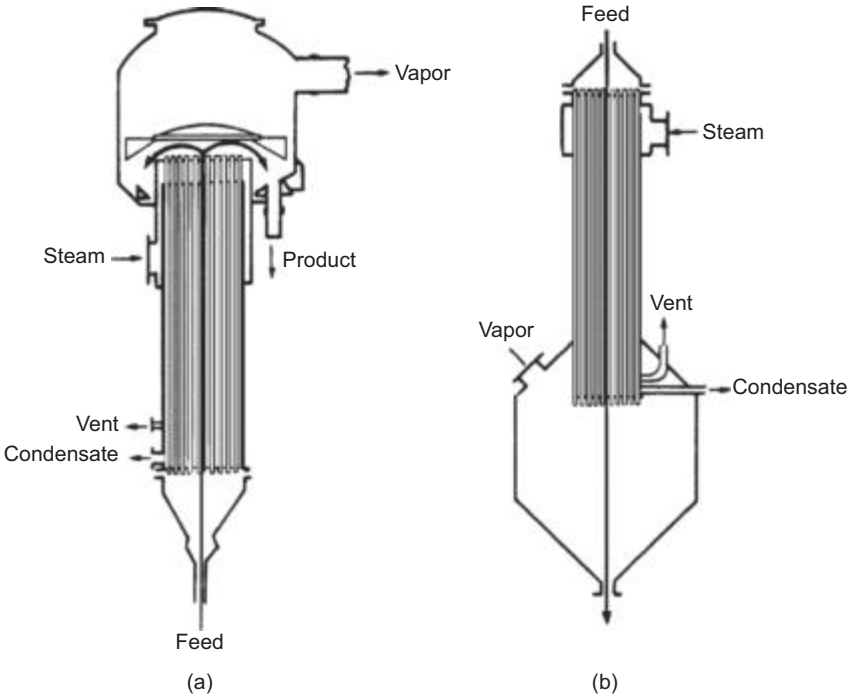


FIG. 16.17 Long-tube evaporators. (a) Rising film. (b) Falling film.

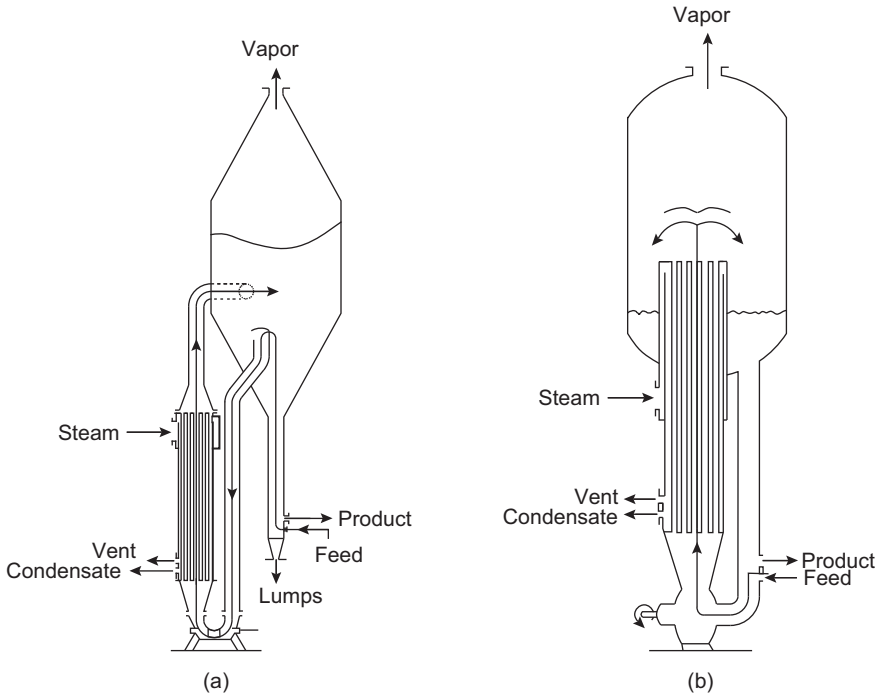


FIG. 16.18 Forced-circulation evaporators. (a) Submerged tube. (b) Boiling tube.

Wiped-film evaporators (Fig. 16.19)

In this design, a thin layer of solution is spread on the heating surface by mechanical means. Wiped-film evaporators are used for very viscous materials and for producing solid products. Wiped-film evaporators are sometimes referred to as agitated thin-film evaporators. The design and applications of this type of evaporator are discussed by Mutzenburg (1965), Parker (1965), and Fischer (1965).

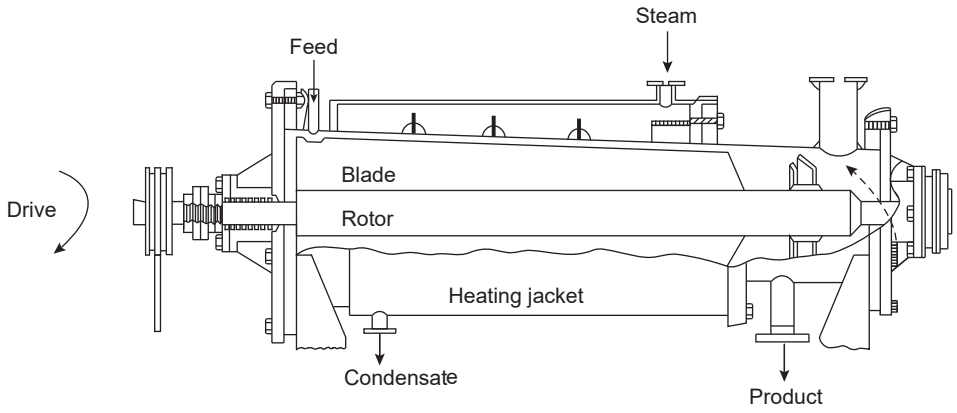


FIG. 16.19 Horizontal wiped-film evaporator.

Short-tube evaporators

Short-tube evaporators, also called callandria evaporators, are used in the sugar industry; see Chhabra and Gurappa (2019).

Evaporator selection

The selection of the most suitable evaporator type for a particular application will depend on the following factors:

1. The throughput required
2. The viscosity of the feed and the increase in viscosity during evaporation
3. The nature of the product required: solid, slurry, or concentrated solution
4. The heat sensitivity of the product
5. Whether the materials are fouling or nonfouling
6. Whether the solution is likely to foam
7. Whether direct heating can be used

A selection guide based on these factors is given in Fig. 16.20; see also Parker (1963).

	Feed conditions							Suitable for heat-sensitive materials
	Viscosity, mN s/m^2							
Evaporator type	Very viscous > 1000	Medium viscosity < 1000 max	Low viscosity < 100	Foaming	Scaling or fouling	Crystals produced	Solids in suspension	
Recirculating Calandria (short vertical tube)		←	—	—	—	—	→	No
Forced circulation		←	—	—	—	→		Yes
Falling film			↔					No
Natural circulation			↔	—				No
Single pass wiped film	←	—	—	—	—	—	→	Yes
Tubular (long tube) Falling film			↔					Yes
Rising film			↔	—				Yes

FIG. 16.20 Evaporator selection guide.

Evaporator design

It can be seen from Figs. 16.17 and 16.18 that most evaporators consist of a shell and tube heat exchanger bundle combined with a vapor–liquid disengaging space. The major cost in these designs is the heat exchange tubes; hence the cost correlations for evaporators are based on surface area; see Table 7.2. The exception is for wiped-film evaporators, which must always be designed and costed in consultation with a vendor.

The heat transfer bundle of an evaporator can be designed using the methods given for boiling heat transfer in Section 19.11. The boiling fluid is always on the tube side, and the hot utility (usually steam) is placed on the shell side.

If the fraction of the feed that is evaporated is greater than about 30%, it may be advantageous to recirculate some of the product to the feed. This increases the liquid flow and gives more uniform heat transfer. When product recirculation is used in food applications, as in the production of condensed milk, care must be taken to ensure that the residence time in the evaporator is not so large as to damage the product or cause fouling of the tubes. The residence time can be estimated from the liquid holdup in the evaporator divided by the product flow rate. The falling-film type has the least liquid holdup and is preferred in food applications.

Auxiliary equipment

Condensers and vacuum pumps will be needed for evaporators operated under vacuum. For aqueous solutions, steam ejectors and jet condensers are normally used. Jet condensers are direct-contact condensers, where the vapor is condensed by contact with jets of cooling water. Indirect, surface condensers are used where it is necessary to keep the condensed vapor and cooling water effluent separate.

Example 16.5

Estimate the heat exchange area required for an evaporator that concentrates 4000 kg/h of apple juice by removing 40% of the water content. Low-pressure steam at 120 °C is available as heat source. The evaporator is run under a slight vacuum, such that the temperature of the boiling apple juice concentrate is maintained at 100 °C.

Solution

For an initial estimate we can assume the properties of apple juice are the same as those of water.

Latent heat of evaporation ~ 2200 kJ/kg at 100°C

Heat exchange duty required $= 4000 \times 0.4 \times 2200/3600 = 978$ kW

Because the fraction of feed evaporated is >30%, we can assume that the evaporator has product recirculation, in which case the tube-side temperature will be approximately constant at 100 °C.

Mean temperature difference $= 120 - 100 = 20$°C

An initial estimate of the heat transfer coefficient can be made using the nomograph in Fig. 19.1, which suggests that an overall heat transfer coefficient of about 1500 W/m^{2}K will be reasonable.

Estimate area:

$$Q = UA\Delta T_m \tag{19.1}$$

where Q = heat transferred per unit time, W
U = the overall heat transfer coefficient, W/m^2°C
A = heat transfer area, m^2
ΔT_m = the mean temperature difference, the temperature driving force, °C

Hence:

$$\text{Area, } A = \frac{978 \times 10^3}{1500 \times 20} = \underline{\underline{32.6 \text{ m}^2}}$$

This estimate can be used to make an initial layout of the heat transfer bundle. The tube-side heat transfer coefficient can then be estimated using the methods given in Section 19.11, and the shell-side coefficient can be estimated using the methods given in Section 19.10 to arrive at a more accurate determination of the required evaporator area. For preliminary design purposes, this estimate would be adequate to generate an initial (Class 4) estimate of the evaporator cost using the correlation given in Table 7.2.

16.5.2 Crystallization

Crystallization is used for the production, purification, and recovery of solids. Crystalline products have an attractive appearance, are free flowing, and are easily handled and packaged. The process is used in a wide range of industries, from the small-scale production of specialized chemicals, such as pharmaceutical products, to the high-tonnage production of commodity products such as sugar, common salt, and fertilizers.

Crystallization theory is covered in Mullin (2019) and Jones (2002). Descriptions of the various crystallizers used commercially can be found in these texts and in handbooks: Mersmann (2001), Myerson et al. (2019), Green and Southard (2018), and Schweitzer (1997). Procedures for the scale-up and design of crystallizers are given by Mersmann (2001) and Mersham (1984, 1988).

Crystallization equipment can be classified by the method used to obtain supersaturation of the liquor and also by the method used to suspend the growing crystals. Supersaturation is obtained by cooling or evaporation. There are four basic types of crystallizer; these are described briefly next.

Tank crystallizers

Tank crystallizers are the simplest type of industrial crystallizing equipment. Crystallization is induced by cooling the mother liquor in tanks, which may be agitated and equipped with cooling coils or jackets. Tank crystallizers are operated batch-wise and are generally used for small-scale production.

Scraped-surface crystallizers

Scraped-surface crystallizers are similar in principle to the tank type, but the cooling surfaces are continually scraped or agitated to prevent fouling by deposited crystals and to promote heat transfer. They are suitable for processing high-viscosity liquors. Scraped-surface crystallizers can be operated batch-wise, with recirculation of the mother liquor, or continuously. A disadvantage of this type is that they tend to produce very small crystals.

Circulating magma crystallizers (Fig. 16.21)

In this type, both the liquor and growing crystals are circulated through the zone in which supersaturation occurs. Circulating magma crystallizers are probably the most important type of large-scale crystallizers used in the chemical process industry. Designs are available in which supersaturation is achieved by direct cooling, evaporation, or evaporative cooling under vacuum.

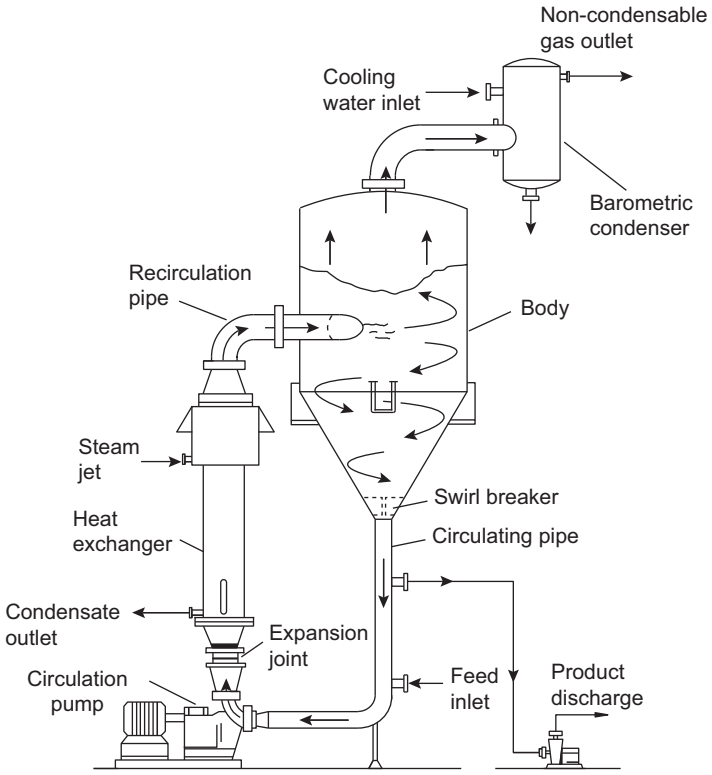


FIG. 16.21 Circulating magma crystallizer (evaporative type).

Circulating liquor crystallizers (Fig. 16.22)

In a circulating liquor crystallizer only the liquor is circulated through the heating or cooling equipment; the crystals are retained in suspension in the crystallizing zone by the up-flow of liquor. Circulating liquor crystallizers produce crystals of regular size. The basic design consists of three components: a vessel in which the crystals are suspended and grow and are removed; a means of producing supersaturation, by cooling or evaporation; and a means of circulating the liquor. The Oslo crystallizer (see Fig. 10.50) is the archetypical design for this type of crystallizing equipment.

Circulating liquor crystallizers and circulating magma crystallizers are used for the large-scale production of a wide range of crystal products. Typical applications of the main types of crystallizers are summarized in Table 16.2; see also Larson (1978).

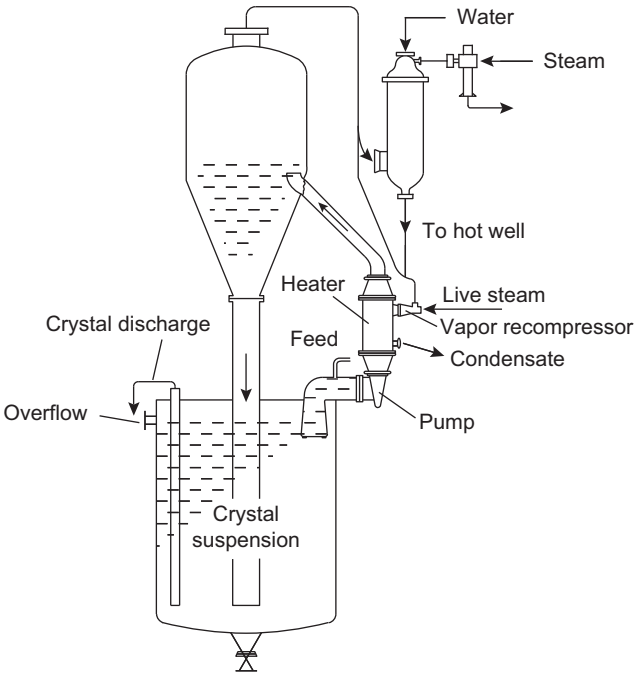


FIG. 16.22 Oslo evaporative crystallizer.

Crystallizer design

Crystallizers are normally sized in consultation with a specialist equipment vendor. The important design parameters are:

1. Process throughput
2. Feed concentration
3. Target solids yield (recovery)
4. Target particle size distribution
5. Product purity (particularly in fractional crystallization)
6. Heat addition or removal requirements, including latent heat as well as sensible heat

The yield of a crystallizer is limited by both solid−liquid equilibrium and the desire to maintain a low enough solids fraction to allow slurry flow of the product. If the solvent is removed by evaporation, the mother liquor can be recycled to the crystallizer after the crystals have been removed by filtration, as long as impurities do not accumulate in the recycle.

TABLE 16.2 Selection of crystallizers

Crystallizer type	Applications	Typical uses
Tank	Batch operation, small-scale production.	Fatty acids, vegetable oils, sugars
Scraped surface	Organic compounds, where fouling is a problem, viscous materials.	Chlorobenzenes, organic acids, paraffin waxes, naphthalene, urea
Circulating magma	Production of large-sized crystals. High throughputs.	Ammonium and other inorganic salts, sodium and potassium chlorides
Circulating liquor	Production of uniform crystals (smaller size than circulating silver magma). High throughputs.	Gypsum, inorganic salts, sodium and potassium nitrates, nitrates

16.5.3 Precipitation

Precipitation can be considered as a branch of crystallization, although the solid phase that is formed need not be crystalline.

The solubility of organic solutes can be influenced by temperature, composition, pH, solvent polarity, and ionic strength. If something is added to the solvent to change one or more of these properties, the solute can sometimes be precipitated out of solution. If the solvent volume is not significantly changed, the recovery of solute is equal to the change in solute solubility divided by the initial solubility:

$$\text{Solute recovery} = \frac{\text{solute precipitated}}{\text{total solute fed}} \approx \frac{\text{initial solubility} - \text{final solubility}}{\text{initial solubility}} \tag{16.11}$$

Precipitation is widely used in the recovery of large organic molecules, such as specialty chemicals, pharmaceutical and food compounds, proteins, and other biological products. Some of the common techniques that are used include:

1. Salting out, in which a salt such as calcium citrate, calcium chloride or ammonium sulfate is added to an aqueous solution to raise the ionic strength and cause precipitation.
2. Changing solution polarity by adding methanol, ethanol, acetone, acetonitrile or other suitable solvent.
3. Changing the pH by adding acid (sometimes known as acidulation) or base.
4. Heat treatment ("cooking") to thermally degrade an unwanted solute that is then precipitated.
5. Adsorption precipitation by adding diatomaceous earth, casein, gelatin, activated carbon, clay, or other large particles that can adsorb the organic species and then settle as precipitate.

Precipitation operations usually do not require evaporation of solvent or cooling of a saturated solution and so can be carried out in simpler equipment than crystallization. The process usually consists of a mixing tank or in-line mixer, followed by a solid–liquid separation device such as a hydrocyclone or centrifuge, as described in Section 18.6.

Precipitation is discussed in detail by Sohnel and Garside (1992).

16.5.4 Membrane separations

Membranes are widely used for concentration of solutions of dissolved solids, as well as suspensions of particulates. A tubular membrane that is permeable to the solvent but not the solute can be used to remove solvent from a solution in the same manner as cross-flow filtration (see Section 18.6.2). These processes are classified as microfiltration, ultrafiltration, or nanofiltration, depending on the size of particulate or molecule that is retained; see Table 16.3. The use of a membrane for solvent removal is usually preferred over solvent evaporation if the solute is sensitive to high temperatures. This is often the case for biologically active large molecules such as proteins and enzymes and for flavor compounds found in foods and beverages.

Membranes can also be found that are selective for the solute over the solvent. Such membranes allow the solute to be transferred to a different solvent without intimate mixing of the solvents, which can be beneficial for solvent or product degradation or when the two solvents are mutually miscible. In the pharmaceuticals industry, the use of solute-selective membranes is known as *diafiltration*, because of the close analogy to dialysis in organisms. A recent variant on diafiltration is to use a charged membrane to increase the selectivity for solute; see Mehta et al. (2008) for a good example.

TABLE 16.3 Membrane filtration process

Process	Approximate size range (m)	Applications
Microfiltration	10^{-8} to 10^{-4}	pollen, bacteria, blood cells
Ultrafiltration	10^{-9} to 10^{-8}	proteins and virus
Nanofiltration	5×10^{-9} to 15×10^{-9}	water softening
Reverse osmosis	10^{-10} to 10^{-9}	desalination
Dialysis	10^{-9} to molecules	blood purification
Electrodialysis	10^{-9} to molecules	separation of electrolytes
Pervaporation	10^{-9} to molecules	dehydration of ethanol
Gas permeation	10^{-9} to molecules	hydrogen recovery, dehydration

When membranes are used for filtration or solute concentration, the limit on solvent recovery is set by the need to avoid fouling or scaling of the membrane and maintain a pumpable slurry. Mass transfer at the membrane wall causes the fluid closest to the membrane to be depleted in solvent; a phenomenon known as concentration polarization. Because the fluid at the membrane wall is depleted in solvent and enriched in solute, precipitation or crystallization can occur if the solute solubility is exceeded. Either of these processes can lead to membrane fouling and loss of throughput. Solvent recovery membranes are therefore usually operated at an outlet concentration well below saturation. Osmotic effects can also decrease the flux through a membrane.

The design of membranes for solute transfer is similar to the design of gas separation membranes, as described in Section 16.2.2, with the exception that a second solvent is usually introduced on the permeate side to remove the solute. Hollow-fiber or tubular membranes are most commonly used.

The design of membrane separations for liquids is discussed in Scott and Hughes (1996), Cheryan (1998), McGregor (1986), Rautenbach and Albrecht (1989), Noble and Stern (1995), Mulder (1996), Porter (1997), Hoffman (2003), Sridhar and Moulik (2018), and Baker (2012). Applications of membranes to biological systems are described in the book by Wang (2001) and the review paper by van Reis and Zydney (2007). The special case of recovery of purified water from salt solutions by reverse osmosis (RO) is discussed next.

Reverse osmosis

Reverse osmosis (RO) is by far the most widely used membrane process. In an RO plant, water passes through a membrane, while dissolved minerals and other solids are rejected in the retentate. Reverse osmosis is used to generate deionized process feed water, purify boiler feed water, recover water from waste streams, and desalinate sea water or brackish water for drinking and irrigation.

In an RO process, the feed water is pressurized to provide an adequate pressure gradient to overcome the difference in osmotic potential between the briny retentate and the purer permeate. Under the applied pressure gradient, water flows through the membrane against the concentration gradient. The membranes are usually designed as spiral-wound modules and are operated in cross-flow; see Section 16.2.2.

Reverse osmosis plants are usually purchased as modular plants designed by one of the major water treatment companies. Cost correlations have been developed and can be found in Aspen Capital Cost Estimator (ACCE), Cleopatra Enterprise, and other cost estimating programs.

The recovery of water from an RO plant depends on the feed water quality, the product specifications, and the need to prevent membrane fouling. Highly pure water is usually not obtained in a single stage. The membrane typically rejects 96% to 98% of the salts per stage, and several stages may be used to achieve the desired purity, with recycle of retentate as described in Section 16.2.2.

As with any solvent-rejection membrane, the designer must ensure that the retentate will not reach concentrations of solute that will cause the membrane to be fouled. Allowance must also be made for concentration polarization near the membrane. At high recovery of water, the osmotic pressure of the solution on the retentate side increases dramatically. The limit on recovery is often set by an economic trade-off between the cost of consuming additional feed and the cost of pumping to a higher pressure. Table 16.4 gives the osmotic pressure of NaCl and sea salt solutions at different concentrations at 40 °C. Some guidelines on membrane fluxes and retentate flows are given by Kucera (2008). A typical product recovery when generating purified water from town water is 50% to 75%, but the recovery depends strongly on the factors described earlier and is often less than 30% in desalination plants.

TABLE 16.4 Osmotic pressure of sea salt and sodium chloride solutions at 40 °C

Molality of NaCl	Osmotic pressure
(mol/kg)	(atm)
0.01	0.49
0.10	4.76
0.50	23.60
1.0	48.08
1.50	73.93
2.00	101.3
3.00	161.6
4.00	230.5
5.00	309.4
Weight % sea salts	Osmotic pressure
(wt%)	(atm)
1.00	7.41
2.00	14.88
3.45*	26.17
5.00	38.96
7.50	61.40
10.00	86.46
15.00	146.6
20.00	225.1
25.00	331

** 3.45 wt% solids is taken as the value for standard sea water.*
From Stoughton and Lietzke, 1965.

When specifying the use of an RO system for process feed water, the design engineer must allow for the cost of the extra feed water that is needed. This is illustrated in Example 16.6.

The performance of RO plants can often be substantially improved by pretreatment of the water feed. Common pretreatment processes include filtration, softening of the water by cation exchange, activated carbon adsorption of chlorine and organics, and addition of chemicals to prevent biological fouling and suppress precipitation.

Because of its widespread use, there is an abundant literature on RO. It is covered in all of the general books on membranes listed earlier and in the specialist books by Amjad (1993), Byrne (2002), Wilf et al. (2007), Kucera (2010), and AWWA (2007). The use of RO for water recovery from waste water is discussed by Aerts and Tong (2009). Good introductory descriptions of the technology are given in the articles by Stover (2014) and Kucera (2019).

Example 16.6

A reverse osmosis plant is to be designed to produce 50 kg/s of boiler feed water with less than 20 ppmw of NaCl starting from sea water that contains 3.5 wt% NaCl. The 40 m^2 membrane modules operate at 60 atm and achieve a flux of 0.4 m^3/m^2.day when the permeate pressure is 2 atm. If each membrane module has a rejection of 96% of the salt fed to it, determine the overall membrane sequence and the water feed rate required.

Solution

Target concentration $= 20$ ppmw $= 0.002$ wt%.

If the permeate pressure is 2 atm and the retentate is at 60 atm, then the pressure drop across the membrane is $60 - 2 = 58$ atm.

From Table 16.4, an osmotic pressure of 58 atm corresponds to a concentration of 7.44 wt%. We need to make an allowance for concentration polarization at the membrane, so assume that the retentate bulk concentration is 70% of this concentration (i.e., 5.21 wt%).

Mass balance on salt across first stage, basis 100 kg/s of feed, 96% rejection of salts:

$$\begin{aligned}\text{Feed} &= \text{Permeate} + \text{Retentate}\\ 3.5 &= 3.5 \times 0.04 + 3.5 \times 0.96\\ &= 0.14 + 3.36\end{aligned}$$

So if the retentate water flow rate is x, then:

$$\frac{3.36}{x+3.36} = 0.0521, \qquad \text{hence } x = \frac{3.36}{0.0521} - 3.36 = 61.1\text{‘kg/s}$$

So, by difference, the water flow in the permeate is $96.5 - 61.1 = 35.4$ kg/s, and the salt concentration in the permeate is $0.14/(0.14 + 61.1) = 0.39$ wt%, which does not meet the target.

If we assume a simple cascade with no retentate recycle, then the second stage can be calculated in the same way:

Salt retained in permeate $= 0.14 \times 0.04 = 0.0056$ kg/s

Salt rejected in retentate $= 0.14 \times 0.96 = 0.1344$ kg/s

Retentate water flow $= \dfrac{0.1344}{0.0521} - 0.1344 = 2.44$ kg/s

Permeate water flow $= 35.4 - 2.44 = 32.94$ kg/s

Permeate salt concentration $= 0.0056/(0.0056 + 32.94) = 0.017$ wt%, which still does not meet the target.

This calculation can be repeated for subsequent stages and is easily coded into a spreadsheet. The third-stage results are:

Salt retained in permeate $= 0.0056 \times 0.04 = 0.000224$ kg/s

Salt rejected in retentate $= 0.0056 \times 0.96 = 0.005376$ kg/s

Retentate water flow $= \dfrac{0.005376}{0.0521} - 0.005376 = 0.098$ kg/s

Permeate water flow $= 32.94 - 0.098 = 32.85$ kg/s

Permeate salt concentration $= 0.000224/(0.000224 + 32.85) = 0.00068$ wt%, which now exceeds the target specification, so a part of the second-stage product can bypass the third stage; however, for design purposes we will assume that all the stages are fully used, as this provides some additional safety factor for fouling, concentration polarization, etc.

The overall recovery of water is 32.85 kg/s out of 96.5 kg/s fed (i.e., 34%), so the feed rate to produce 50 kg/s of RO water is $50/0.34 = 147$ kg of water. Allowing for the salt in the feed, we also have $147 \times 0.035/(1 - 0.035) = 5.33$ kg/s of salt, so the total feed is 152 kg/s of sea water.

Note that the retentate flow in the third stage has become very small. This is not a practical value, and a higher flow rate would be necessary. A higher flow rate can be accomplished by reducing the outlet retentate concentration and recycling the retentate to an earlier point in the network (see Fig. 16.10c). The network with recycles is more difficult to solve using hand calculations, but can easily be modeled using process simulation software. If the process simulation program does not have a membrane unit operation, then the RO membrane can be modeled as a fixed-split separator; see Section 4.5.3.

By examination of the permeate flows calculated earlier, we see that the permeate flow is essentially unchanged and roughly 32.9 kg/s from stage 2 onwards (≈50 kg/s on the design flow rate basis). The permeate from stage 1 is 35.4 kg/s, which when corrected to the 50 kg/s production basis would be $35.4 \times 152/100 = 53.8$ kg/s. So if we allow roughly 10% additional flow (relative to product rate) in each stage for recycles, then we can assume 59.2 kg/s flow in each stage:

$$59.2 \text{ kg/s} = \frac{59.2 \times 3600 \times 24}{1000} = 5114 \text{ m}^3\text{/day}$$

So if each 40 m^2 membrane module permeates 0.4 m^3/m^2.day, then the total number of modules per stage:

$$= \frac{5114}{40 \times 0.4} = 320$$

Hence the total number of modules $= 320 \times 3 = 960$.

With some allowance for spare modules, the sequence is then three stages, each containing 330 modules, with roughly 10% recycle from stages 2 and 3. These results would need to be confirmed by detailed simulation and discussion with a vendor.

16.5.5 Ion exchange

Ion exchange is used for water softening, demineralization and separation and recovery of salts, including salts of organic acids and bases. In an ion exchange process, the solution flows through a bed of resin beads. The resin is a polymer that has been functionalized by the addition of either acidic or basic groups. For example, sulfonated polystyrene contains $-SO_3^-$ groups that attach to cations from the solution, and hence can be used as a cation exchange resin. The particular choice of acidic or basic groups allows the designer to modify the strength of interaction and hence the selectivity of the resin.

When a solution is passed over a cation exchange resin, the cations in the solution equilibrate with the cations that were attached to the resin, and hence effectively become adsorbed onto the resin. When the resin nears breakthrough, it can be regenerated by washing with a solution of counter-ion: typically H^+, Na^+, or Ca^{2+} for cation exchange or Cl^-, HO^-, or NO_3^- for anion exchange.

Full deionization can be accomplished by carrying out cation exchange using H^+ as the counter-ion, followed by anion exchange using HO^- as the counter-ion.

The most common ion exchange process is water softening, in which Ca^{2+} and Mg^{2+} that occur naturally in hard water are exchanged with Na^+ using a cation exchange resin that is regenerated with NaCl. Water softening is used for boiler feed water and to prepare water for RO units. Small units are also used for domestic water softening in regions that have high water hardness.

The capacity of an ion exchange resin depends on the extent of functionalization of the polymer and is normally expressed in mmol/g or mmol/mL of resin. The units millimoles (mmol) are sometimes written as milliequivalents (meq). For cation exchange resins, the loading is per g or mL of dry hydrogen-form resin, and for anion exchange resins it is usually per g or mL of dry chlorine-form resin. Capacities for some of the more commonly used resins are given in Green and Southard (2018). A rough estimate of the total bed volume required can be made by assuming that the bed operates to 70% of breakthrough; a more detailed analysis would usually be made by a specialist designer.

As with adsorption (see Section 16.2.1), a continuous ion-exchange system requires at least two beds of resin, so that one can be in regeneration while the other is in process service.

When specifying an ion-exchange system, the design engineer must allow for the regenerant and effluent treatment systems. The regenerant is a salt of the counter-ion, usually in aqueous solution. The regenerant is required in an amount that is somewhat greater than the stoichiometric equivalent of the exchanged ion to provide an adequate difference in chemical potential to drive the exchanged ion off the resin and ensure that regeneration is completed. A good initial estimate is 150% to 200% of the stoichiometric equivalent. The regenerant is often fed at high concentration to minimize the amount of effluent formed during regeneration. The spent regenerant may require neutralization or other additional treatment before it can be sent to a wastewater plant.

Many pharmaceutical products and intermediates are organic salts that can be recovered by ion exchange. If the ion loaded on the resin is the desired product, then the regenerant should be chosen to give the product in a suitable form for further processing.

An introduction to the theory of ion exchange is given in Chhabra and Gurappa (2019). A more detailed discussion of the technology is given in the book by Helfferich (1995). Wachinski (2016) discusses the application of ion exchange to waste recovery.

Example 16.7

Thiocyanate ions can be removed from sodium carbonate/bicarbonate solution that is used for oxidative scrubbing of H_2S using a moderately basic anion exchange resin (see US 4,999,113). The flow rate of the scrubbing solution is 40 m^3/h, and the initial concentration of thiocyanate is 10 g/l. A polystyrene-based anion exchange resin suitable for this duty has capacity of 1.8 eq/L. The resin can be regenerated by flushing 1.5 equivalents of 4.0 wt% NaOH, preceded by the same volume of water. Two beds are used, with one in operation and one in regeneration. If the bed is designed to be 80% loaded at the end of a 2-hour operation cycle, estimate the bed volume. Also determine the flow rate of sodium hydroxide required during the regeneration.

Solution

After 2 hours, the amount of thiocyanate exchanged $= 40 \times 10 \times 2 = 800$ kg

Thiocyanate is SCN^-, so has a molecular weight $= 32 + 12 + 14 = 58$ g/mol

Molar loading $= 800/58 = 13.79$ kmol

Bed volume required for complete loading $= 13.79/1.8 = 7.66\ m^3$

So bed volume for 80% loading at end of 2 hours $= 7.66/0.8 = \underline{\underline{9.58\ m^3}}$

If this were designed as a 4:1 cylindrical vessel, then volume $= \pi D_v^3$, so vessel diameter would be $= 1.45$ m and height $= 5.8$ m, allowing the vessels to be designed, sized, and costed using the methods given in Chapter 14.

100 kg of 4.0 wt% NaOH has 4 kg of NaOH; hence $4 \times (17/40) = 1.7$ kg of HO^- anions

1.7 kg of $HO^- = 1700/17 = 100$ mol, so 4 wt% NaOH is 1 mol/kg

9.58 $m^3$of resin has capacity $9.58 \times 1.8 = 17.24$ kmol

So, flush requires 1.5 equivalents $= 1.5 \times 17.24 = 25.87$ kmol, which must be completed in 1 hour (to allow for the preceding 1-hour flush with the same volumetric flow rate of water). Hence the flow rate of 4.0 wt% sodium hydroxide solution must be $\underline{\underline{25.87 \times 10^3}}$ kg/hr.

Note that the regeneration flow rate is less than the process flow rate, as a more concentrated solution is used for the regeneration.

16.5.6 Solvent extraction and leaching

Solvent extraction (liquid–liquid extraction)

Solvent extraction, also called liquid–liquid extraction, can be used to separate a substance from a solution by extraction into another solvent. It can be used either to recover a valuable substance from the original solution or to purify the original solvent by removing an unwanted component. Examples of solvent extraction are the extraction of uranium and plutonium salts from solution in nitric acid in nuclear fuel reprocessing using kerosene as solvent and the extraction of benzene from reformed naphtha using sulfolane as solvent.

The process depends on the substance being extracted, the solute, having a greater solubility in the solvent used for the extraction than in the original feed solvent. The two solvents must be essentially immiscible.

The solvents are mixed in a contactor to effect the transfer of solute, and then the phases are separated. The depleted feed solvent leaving the extractor is called the raffinate, and the solute-rich extraction solvent, the *extract*. The solute is normally recovered from the extraction solvent by distillation, and the extraction solvent recycled.

The simplest form of extractor is a mixer-settler, which consists of an agitated tank and a decanter. For multistage extraction processes, liquid–liquid contacting columns are used. The design of extraction columns is discussed in Chapter 17, Section 17.16. See also Chhabra and Gurappa (2019), Treybal (1963), Couper et al. (2012), and Green and Southard (2018).

Leaching

Liquids can be extracted from solids by leaching. As the name implies, the soluble component contained in a solid is leached out by contacting the solid with a suitable solvent. A principal application of leaching is in the extraction of valuable oils from nuts and seeds such as palm oil and rapeseed oil.

The equipment used to contact the solids with the solvent is usually a special design to suit the type of solid being processed and is to an extent unique to the particular industry. General details of leaching equipment are given in Green and Southard (2018).

The leaching is normally done using a number of stages. In this respect, the process is similar to liquid–liquid extraction, and the methods used to determine the number of stages required are similar.

For a detailed discussion of the procedures used to determine the number of stages required for a particular process, see Prabhudesai (1997).

16.5.7 Adsorption

Fixed beds of adsorbent are occasionally used for removing small amounts of dissolved solids or liquids from a liquid stream. Common adsorbents are silica, alumina, activated carbon, zeolites, and clays.

When removing a dissolved solid, the process is usually treated as irreversible adsorption; see Section 16.2.1. Reversible adsorption of dissolved components with regeneration of the sorbent using a different solvent is a form of chromatography and is discussed in the following section.

16.5.8 Chromatography

The term chromatography is broadly applied to separation processes in which a fluid is separated into components by passing it over a bed of adsorbent in a continuous flow of carrier fluid. Gas chromatography (GC) is widely used as an analytical method, but is only rarely used for product recovery because of the high-volume flow rates and pressure drop requirements. Liquid-phase chromatography, on the other hand, is extensively used for product recovery and purification, particularly for fine chemicals and biological products; see Harrison (2014).

Most chromatographic separations are carried out in batch or semi-batch mode, but continuous chromatography can be carried out using flow schemes such as simulated moving bed (SMB) chromatography, described later.

The general principles of chromatography are discussed by Ruthven (1984), Ganetsos and Barker (1992), Chhabra and Gurappa (2019), Harrison (2014), and Hagel et al. (2007).

Chromatographic separations rely on different components in the feed having different adsorption equilibria with the solid phase. The solid-phase material can be an inorganic or organic adsorbent, resin, or gel, and is sometimes referred to as the *stationary phase*. The liquid phase is called the mobile phase and consists of the feed liquid, as well as the carrier liquid, which is also sometimes called the eluent or desorbent. The process performance is strongly influenced by the choice of stationary phase and mobile phase.

Batch chromatography

Batch chromatography processes operate in a similar mode to laboratory-scale chromatography. They are consequently favored by chemists for preparative chromatography and smaller-scale production chromatography, as the scale-up from lab methods is more straightforward than for continuous chromatography.

In batch chromatography, a pulse of feed is injected into a continuously flowing stream of mobile phase that passes over a long column packed with a suitable stationary phase, as shown in Fig. 16.23(a). The more strongly adsorbed species pass through the column more slowly than less strongly adsorbed species. If a long enough column is used, then the different species can be resolved into fractions (or "peaks") that are enriched in different components of the feed (see Fig. 16.23b). If the column effluent composition is monitored, the first fractions recovered will contain material that adsorbs less strongly than the desired product ("lights"). This material can be sent for eluent recovery or discarded as waste. The next fractions are rich in product and are sent to product recovery. Finally, material that is more strongly adsorbed than the desired product ("heavies") is eluted, and this material is also sent to solvent recovery or waste disposal.

If all the material can be desorbed from the column within a reasonable time and carrier flow rate, the column is then clean enough to accept a new injection of feed, and the process is repeated. Occasionally, the cost in time and desorbent to recover the heavier material is greater than the cost of emptying the column and reloading with fresh stationary phase, in which case the cycle is ended after collection of the product and the spent stationary phase is sent to waste disposal.

The eluent can be recovered from the product and waste streams and recycled to the feed; however, in many fine chemical and pharmaceutical processes, the spent solvent is discarded or sold as a by-product to eliminate concerns about components accumulating in the solvent recycle.

Batch chromatography columns can be designed as dynamic processes or by using an equilibrium stage analogy; see Chapter 8 of Ruthven (1984).

When a batch column is scaled up to a larger diameter, there will be greater dispersion of the components, leading to broader peaks, and hence the column length must be increased. Batch chromatography is therefore inefficient in the use of stationary phase, particularly if the stationary phase is discarded frequently. When very long columns are used, the pressure drop can be very high; hence the process is sometimes known as high-pressure liquid chromatography or high-performance liquid chromatography (HPLC).

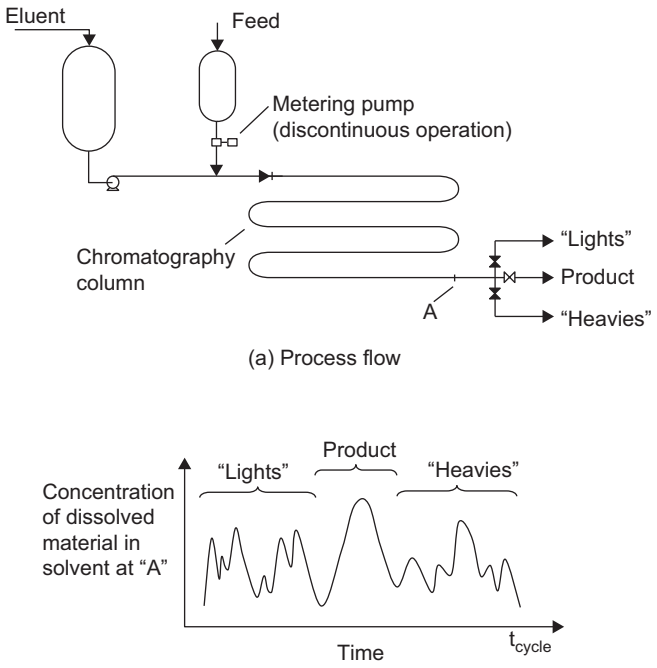


FIG. 16.23 Batch chromatography.

Gel permeation chromatography

Gel permeation chromatography is a variation of batch chromatography. The stationary phase is selected to have a pore structure that excludes the desired product. The larger molecules that cannot enter the pores are eluted first, and smaller molecules are eluted later. The separation order is thus reversed from typical batch chromatography. With gel permeation chromatography, it is much easier to completely regenerate the sorbent, and the cycle time can be reduced. Other aspects of the design are similar to conventional batch chromatography.

Affinity chromatography

Affinity chromatography is probably the most widely used preparative and production chromatography method in industry, particularly for recovery of biochemicals and large molecules.

In affinity chromatography, the stationary phase is selected or designed to have a highly specific interaction with the desired component. Commonly used interactions include enzyme−inhibitor, antibody−antigen, and lectin−cell wall. For example, monoclonal antibodies (mAb) can be synthesized that have very highly specific binding to a desired protein. If the mAb is chemically bound to beads of agarose, polyacrylamide, or other suitable material, the beads can be used to pack a column with specific selectivity for the target protein.

Affinity chromatography is in many respects more like an adsorption−desorption process (Section 16.2.1) or an ion exchange process (Section 16.5.5) than a chromatography process. The feed liquid can be passed through the bed without requiring additional eluent. The high selectivity of the stationary phase allows the bed to be kept on stream until the sorbent is fully loaded or nearly fully loaded. The sorbent is then regenerated by the eluent flow. The regeneration step usually involves a change in solvent properties to disrupt the affinity between the sorbent and adsorbed species, for example, a change in solvent polarity, pH, ionic strength, or occasionally even temperature. When multiple species are adsorbed, the eluent properties may be changed over time so that different species are eluted in sequence. This is known as applying a solvent gradient.

The design of affinity chromatography columns is similar to the design of ion exchange columns, as illustrated in Example 16.7. The volume of stationary-phase media is determined by the capacity of the media, the feed concentration and flow rate, and the desired time between regenerations. In batch processes, the operating cycle will usually be chosen to allow the column to be loaded, regenerated, and reconditioned within the process cycle time.

One of the most widely used forms of affinity chromatography is protein A chromatography, which can be used to purify a wide range of MAb and can achieve product purities higher than 99%. Applications and limitations of protein A chromatography are described by Shukla et al. (2007).

The cost of an affinity chromatography packing is usually much greater than the cost of conventional chromatography media, even though the adsorbent is used more efficiently and column sizes are generally smaller. The column is therefore more likely to be fully regenerated so that the stationary phase can be reused. Even so, the sorbent performance usually deteriorates over multiple cycles, and stationary-phase replacement can be a significant consumable cost in biochemical and pharmaceutical processes. For example, Follman and Fahrner (2004) state that protein A affinity chromatography accounts for 35% of the downstream purification costs for mAb production, although the cost of production of mAb is usually a small fraction of the sales price (Kelley, 2009).

A good introduction to affinity chromatography is given in the book by Mohr and Pommerening (1986). More recent work is described in Ganetsos and Barker (1992) and Hagel et al. (2007).

Continuous chromatography

A truly continuous chromatography process would employ countercurrent flow of the solid phase and the desorbent, as shown in Fig. 16.24(a). If the liquid feed is introduced at a height h_F above the base and desorbent liquid is introduced at the top, then a component that is more strongly adsorbed on the sorbent will tend to move up the column with the solid phase, giving the composition profile labeled A in Fig. 16.24(b). Conversely, the component or components that are less strongly adsorbed will tend to move down the column with the desorbent, giving a concentration profile like that labeled B in Fig. 16.24(b). At height h_E, above the feed point, the liquid phase is substantially free of component B, and a product stream containing only desorbent and A can be withdrawn. This stream is known as the extract. Similarly, at height h_R, below the feed point, all of component A has been adsorbed by the solid, and a liquid stream containing only desorbent and B can be recovered. This stream is known as the raffinate.

Above h_E, in the region labeled zone I, the desorbent flow washes A off the solid phase, regenerating a clean sorbent that can be recycled to the bottom of the column. Likewise, below h_R, in the region labeled zone IV, the adsorbent adsorbs remaining B from the liquid, generating a clean desorbent that can be recycled to the top of the column. In practice, this bottom zone is not always used, as it is often cheaper to separate B from desorbent by other methods such as distillation or crystallization.

A true countercurrent continuous chromatography process is analogous to a series of absorbers and strippers:

Zone I: desorption (stripping) of A
Zone II: desorption of B
Zone III: adsorption (absorption) of A, desorption of B
Zone IV: adsorption of B

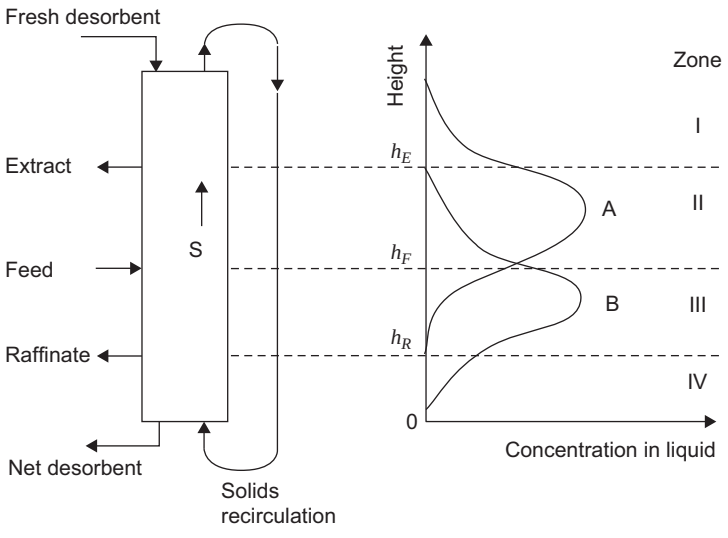


FIG. 16.24 Continuous countercurrent chromatography.

If the equilibrium constants are known, then the process can be approximately modeled in terms of theoretical stages using the Kremser equations or McCabe Thiele analysis; see Ruthven (1984).

A true moving-bed countercurrent chromatography process ("hypersorption") was commercially demonstrated by Dow Chemical and Union Oil Co. in 1947; see Kehde et al. (1948). Unfortunately, most good sorbents are not strong enough to withstand circulation at high solids flow rates and suffer unacceptably high attrition, so this process is no longer practiced.

Instead of circulating the sorbent, the movement of solids can be simulated by using a large number of beds and periodically switching the bed location at which the net flows (feed, extract, raffinate, and desorbent) are fed or removed. In the UOP Sorbex process, illustrated in Fig. 16.25, this is accomplished using a rotary valve; however, the same effect can be obtained using a large number of solenoid switching valves. When the rotary valve is moved to the next position, the net flow that was moving through the pipe between beds n and $n+1$ is switched to move through the pipe between beds $n+1$ and $n+2$. Bed n thus effectively becomes bed $n-1$ relative to the net flows, and movement of the bed is simulated.

Although the solid phase undergoes periodic discrete movement rather than continuous movement relative to the liquid and a steady state is never really established, the performance is nonetheless close to that of true countercurrent chromatography; see Ruthven (1984) and Menet and Thibaut (1999).

Simulated moving bed (SMB) chromatography can be used to obtain products with high purity and high recovery if a suitable combination of sorbent and desorbent can be found. The desorbent can be a solvent or a liquid that has similar adsorption properties to the target molecule and competes for sorbent sites. The sorbent is used much more efficiently than in batch chromatography, and the production rate per kg of sorbent is usually much higher.

Although SMB chromatography has been highly successful in a number of applications, its use is not as widespread as affinity chromatography. The development and scale-up of SMB processes can be tricky, as the ratio of liquid to solid flow rates in each zone has to be chosen to give the desired adsorption or desorption for that zone; see Mazzotti et al. (1997) and Jupke et al. (2002). If the effective stripping factor or absorption factor is too close to 1.0, then a large number of effective stages is needed, or separation will be poor. It is also much more difficult to apply a solvent gradient or vary solvent properties in an SMB process. Because of its higher process development costs, SMB chromatography tends to only be applied to products that are produced in high volume or that require a large amount of expensive sorbent. The largest applications are in recovery of paraxylene from mixed xylenes and

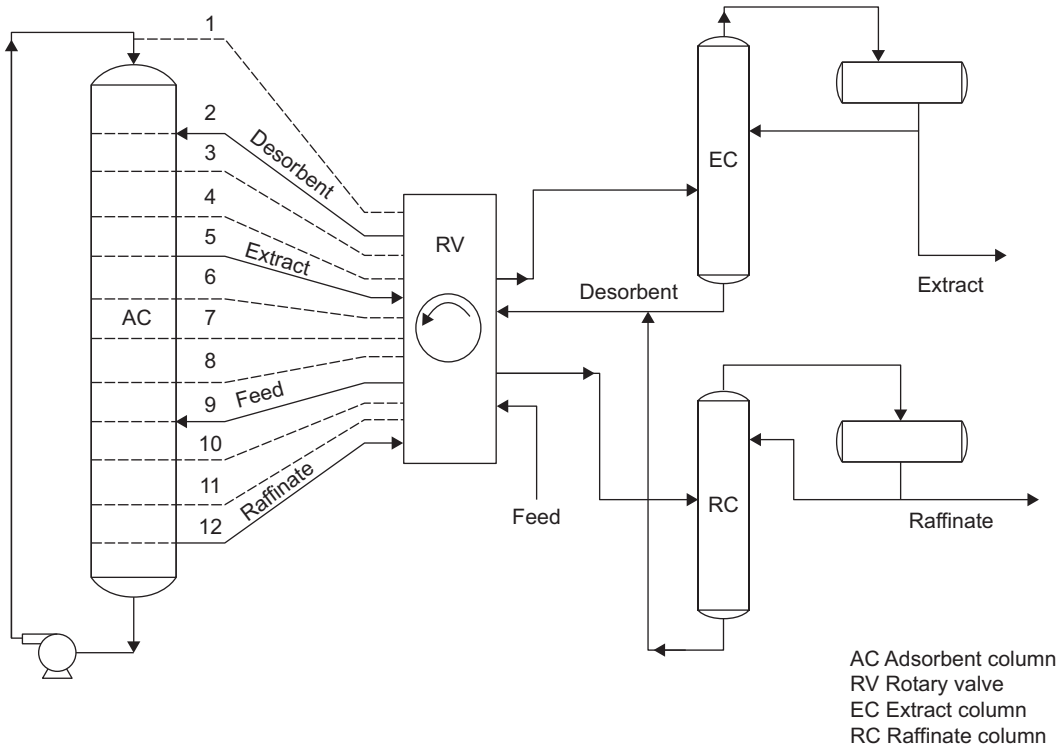


FIG. 16.25 UOP Sorbex process. (Reproduced with permission of UOP, LLC.)

production of high-fructose corn syrup, see Ruthven (1984) and Meyers (2016). There has also recently been a significant expansion in application of SMB chromatography to separation of enantiomers in the pharmaceutical industry, where the high product price and high recovery can justify the added development costs.

16.6 References

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16.7 Nomenclature

		Dimensions in MLT
A	Heat transfer area	$\mathbf{L}^2$
A_i	Area of interface	$\mathbf{L}^2$
Av	Area for vapor flow	$\mathbf{L}^2$
D_T	Tank or vessel diameter	**L**
Dv	Minimum vessel diameter for separator	**L**
d_d	Droplet diameter	**L**
F_1	Feed molar flow rate	$\mathbf{MT}^{-1}$
F_2	Product molar flow rate	$\mathbf{MT}^{-1}$
f_L	Fraction of bed that is fully loaded at end of adsorption phase of cycle	—
f_v	Fraction of cross-sectional area occupied by vapor	—
g	Gravitational acceleration	$\mathbf{LT}^{-2}$

		Dimensions in MLT
h_E	Height of extract draw above base in continuous chromatography	**L**
h_F	Height of feed above base in continuous chromatography	**L**
h_L	Liquid depth	**L**
h_R	Height of raffinate draw above base in continuous chromatography	**L**
hv	Height above liquid level	**L**
k	Equilibrium constant for adsorption	$\mathbf{M}^{-n}\mathbf{L}^{n}\mathbf{T}^{2n}$
L_c	Continuous phase volumetric flow-rate	$\mathbf{L}^{3}\mathbf{T}^{-1}$
L_m	Length of membrane	**L**
Lv	Length of separator, vessel tangent-to-tangent length	**L**
l	Length of decanter vessel	**L**
M_a	Mass of adsorbent per bed	**M**
M_i	Molar flux of component i	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$
$M_{i,ave}$	Average molar flux of component i	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$
M_w	Molecular weight of adsorbed component	—
m	Adsorbent loading, g/g adsorbent	—
m_1	Maximum adsorbent loading (g/g adsorbent)	—
m_2	Minimum adsorbent loading (g/g adsorbent)	—
n	Exponent in equation 16.1	—
P_i	Permeability of membrane for component i (mol/m.s.bar)	**T**
P	Partial pressure of adsorbed component	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
$p_{i,f}$	Local partial pressure of component i on feed side	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
$p_{i,p}$	Local partial pressure of component i on permeate side	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
Q	Heat transferred in unit time	$\mathbf{ML}^{2}\mathbf{T}^{-3}$
r	Radius of decanter vessel	**L**
S_{ij}	Selectivity of a membrane for component i over component j	—
T	Temperature	$\boldsymbol{\theta}$
ΔT_m	Mean temperature difference	$\boldsymbol{\theta}$
t_a	Time an adsorption bed is in the adsorption stage of the cycle	**T**
t_B	Breakthrough time	**T**
U	Overall heat-transfer coefficient	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
u_c	Velocity of continuous phase in a decanter	$\mathbf{LT}^{-1}$
u_d	Settling (terminal) velocity of dispersed phase in a decanter	$\mathbf{LT}^{-1}$
u_s	velocity in a separator	$\mathbf{LT}^{-1}$
u_t	Settling velocity	$\mathbf{LT}^{-1}$
u_v	Maximum allowable vapor velocity in a separating vessel	$\mathbf{LT}^{-1}$
Vv	Gas, or vapor volumetric flow-rate	$\mathbf{L}^{3}\mathbf{T}^{-1}$
w	Width of interface in a decanter	**L**
x	Length	**L**
y_1	Feed mole fraction of adsorbed component	—

		Dimensions in MLT
y_2	Product mole fraction of adsorbed component	—
z	Height of the interface from the base of the vessel	**L**
z_1	Height to light liquid overflow from a decanter	**L**
z_2	Height to heavy liquid overflow from a decanter	**L**
z_3	Height to the interface in a decanter	**L**
δ	Membrane thickness	**L**
μ	Liquid viscosity	$\mathbf{ML^{-1}T^{-1}}$
μ_c	Viscosity of continuous phase	$\mathbf{ML^{-1}T^{-1}}$
ρ	Liquid density	$\mathbf{ML^{-3}}$
ρ_c	Density of the continuous phase	$\mathbf{ML^{-3}}$
ρ_d	Density of the dispersed phase	$\mathbf{ML^{-3}}$
ρ_L	Liquid density	$\mathbf{ML^{-3}}$
ρ_v	Vapor density	$\mathbf{ML^{-3}}$
ρ_1	Light liquid density in a decanter	$\mathbf{ML^{-3}}$
ρ_2	Heavy liquid density in a decanter	$\mathbf{ML^{-3}}$

16.8 Problems

16.1 An electronics plant uses an adsorption system to recover solvent from a vent gas stream and prevent volatile organic compound (VOC) emissions. The vent gas flow rate is 20 m^3/s of dry air at 293 K, 1.5 atm. The initial solvent loading is 1.5 mol%, which must be reduced to 20 ppm to comply with emissions permits. Activated carbon is used as adsorbent and has a capacity of 20 mol/kg of adsorbent and a heat of adsorption of 8 kcal/mol solvent. The sorbent can be regenerated by raising the temperature to 363 K. Design a suitable TSA system for this process. Estimate the amount of adsorbent needed, the vessel volumes, and the minimum regenerant heat requirement for your design. The activated carbon adsorbent has average bulk density 120 kg/m^3 and heat capacity 0.7 J/g.°C. The solvent flammability limits in air are 2.5 to 12.0 vol% at 293 K and 1.2 to 16.0 vol% at 363 K.

16.2 It has been suggested that carbon dioxide can be recovered from flue as using a membrane process. The flue gas has the following composition: nitrogen 73.9 mol%, oxygen 3.1 mol%, carbon dioxide 7.7 mol%, water vapor 15.3 mol%. Using the data in Table 16.1, determine the best membrane material for this process. What are the advantages and disadvantages of the proposed membrane process?

16.3 In a process for the production of acrylic fibers by the emulsion polymerization of acrylonitrile, the unreacted monomer is recovered from water by distillation. Acrylonitrile forms an azeotrope with water, and the overhead product from the column contains around 5 mol% water. The overheads are condensed and the recovered acrylonitrile separated from the water in a decanter. The decanter operating temperature will be 20 °C.
Size a suitable decanter for a feed rate of 3000 kg/h.

16.4 In the production of aniline by the hydrogenation of nitrobenzene, the reactor products are separated from unreacted hydrogen in a condenser. The condensate, which is mainly water and aniline, together with a small amount of unreacted nitrobenzene and cyclohexylamine, is fed to a decanter to separate the water and aniline.

The separation will not be complete, as aniline is slightly soluble in water, and water in aniline. A typical material balance for the decanter is given here:

Basis 100 kg feed

	feed	aqueous stream	organic stream
water	23.8	21.4	2.4
aniline	72.2	1.1	71.1
nitrobenzene	3.2	trace	3.2
cyclohexylamine	0.8	0.8	trace
total	100	23.3	76.7

Design a decanter for this duty for a feed rate of 3500 kg/h. Concentrate on the separation of the water and aniline. The densities of water–aniline solutions are given in Appendix F, Problem F.8, available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793. The decanter will operate at a maximum temperature of 30 °C.

16.5 Water droplets are to be separated from air in a simple separation drum. The flow rate of the air is 1000 m^3/h, at s.t.p., and it contains 75 kg of water. The drum will operate at 1.1 bara pressure and 20 °C.
Size a suitable liquid–vapor separator.

16.6 The vapor from a chlorine vaporizer will contain some liquid droplets. The vaporizer consists of a vertical, cylindrical, vessel with a submerged bundle for heating. A vapor rate of 2500 kg/h is required, and the vaporizer will operate at 6 bara. Size the vessel to restrict the carryover of liquid droplets. The liquid hold-up time need not be considered, as the liquid level will be a function of the thermal design.

CHAPTER

17

Separation columns (distillation, absorption, and extraction)

KEY LEARNING OBJECTIVES

- How to design distillation columns
- How to size distillation columns and select and design distillation column trays
- How to design distillation columns using packing instead of trays
- How to design absorption and stripping columns
- How to design liquid–liquid extraction columns

17.1 Introduction

This chapter covers the design of separating columns. Though the emphasis is on distillation processes, the basic construction features, and many of the design methods, also apply to other multistage processes, such as stripping, absorption, and extraction. Only a brief review of the fundamental principles that underlie the design procedures will be given; a fuller discussion can be found in Chhabra and Gurappa (2019) and in other textbooks: King (1980), Hengstebeck (1976), Kister (1992), Doherty and Malone (2001) and Luyben (2013).

Distillation is probably the most widely used separation process in the chemical and allied industries; its applications ranging from the rectification of alcohol, which has been practiced since antiquity, to the fractionation of crude oil. A good understanding of methods used for correlating vapor–liquid equilibrium data is essential to the understanding of distillation and other equilibrium-staged processes; this subject was covered in Chapter 4.

In recent years, much of the work done to develop reliable design methods for distillation equipment has been carried out by a commercial organization, Fractionation Research, Inc. (FRI), an organization set up with the resources to carry out experimental work on full-size columns. Because their work is proprietary, it is not published in the open literature and it has not been possible to refer to their methods in this book. Fractionation Research's design manuals will, however, be available to design engineers whose companies are subscribing members of the organization. FRI has also produced an excellent training video that shows the physical phenomena that occur when a plate column is operated in different hydraulic regimes. This video can be ordered from FRI at www.fri.org.

Distillation column design

The design of a distillation column can be divided into the following steps:

1. Specify the degree of separation required: set product specifications.
2. Select the operating conditions: batch or continuous; operating pressure.
3. Select the type of contacting device: plates or packing.

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4. Determine the stage and reflux requirements: the number of equilibrium stages.
5. Size the column: diameter, number of real stages.
6. Design the column internals: plates, distributors, packing supports.
7. Mechanical design: vessel and internal fittings.

The principal step is to determine the stage and reflux requirements. This is a relatively simple procedure when the feed is a binary mixture but can be complex when the feed contains more than two components (multicomponent systems).

Almost all distillation design is carried out using commercial process simulation software, as introduced in Chapter 4. The process simulation programs allow the designer to determine the stage and reflux requirements that are needed to attain the desired separation and then size the column and design the column internals. Once the column size is known, the shell can be designed as a pressure vessel (see Chapter 14) and the condenser and reboiler can be designed as heat exchangers (see Chapter 19). The whole design can then be costed and optimized. An example of distillation column optimization was given in Chapter 12.

17.2 Continuous distillation: Process description

The separation of liquid mixtures by distillation depends on differences in volatility between the components. The greater the relative volatilities, the easier is the separation. The basic equipment required for continuous distillation is shown in Fig. 17.1. Vapor flows up the column and liquid flows countercurrently down the column. The vapor and liquid are brought into contact on plates or packing. Part of the condensate from the condenser is returned to the top of the column to provide liquid flow above the feed point (reflux), and part of the liquid from the base of the column is vaporized in the reboiler and returned to provide the vapor flow.

In the section below the feed, the more volatile components are stripped from the liquid, and this is known as the *stripping section*. Above the feed, the concentration of the more volatile components is increased, and this is called the enrichment, or more commonly, the *rectifying section*. Fig. 17.1(a) shows a column producing two product streams, referred to as *distillate* and *bottoms*, from a single feed. Columns are occasionally used with more than one feed and with side streams withdrawn at points up the column (see Fig. 17.1b). This does not alter the basic operation, but complicates the analysis of the process, to some extent.

If the process requirement is to strip a volatile component from a relatively nonvolatile solvent, the rectifying section may be omitted, and the column would then be called a *stripping column*.

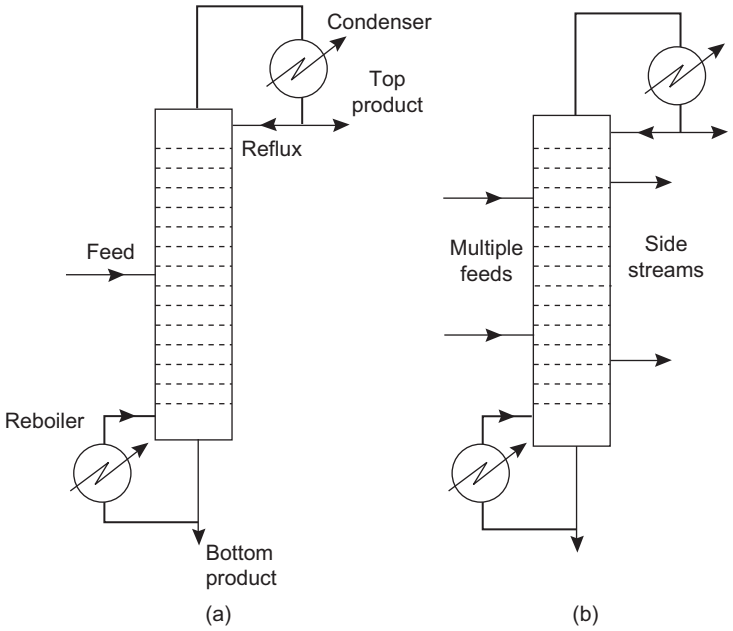


FIG. 17.1 Distillation column. (a) Basic column. (b) Multiple feeds and side streams.

In some operations, where some or all of the top product is required as a vapor, only sufficient liquid is condensed to provide the reflux flow to the column, and the condenser is referred to as a partial condenser. When the liquid is totally condensed, the liquid returned to the column will have the same composition as the top product. In a partial condenser the reflux will be in equilibrium with the vapor leaving the condenser. Virtually pure top and bottom products can be obtained in a single column from a binary feed if no azeotrope is formed, but where the feed contains more than two components, only a single "pure" product can be produced, either from the top or bottom of the column. Several columns will be needed to separate a multicomponent feed into its constituent parts.

17.2.1 Reflux considerations

The reflux ratio, R, is normally defined as:

$$R = \frac{\text{flow returned as reflux}}{\text{flow of top product taken off}}$$

The number of stages required for a given separation will depend on the reflux ratio used.

In an operating column, the effective reflux ratio will be increased by vapor condensed within the column due to heat leakage through the walls. With a well-lagged column, the heat loss will be small, and no allowance is normally made for this increased flow in design calculations. If a column is poorly insulated, changes in the internal reflux due to sudden changes in the external conditions, such as a sudden rain storm, can have a noticeable effect on the column operation and control.

Total reflux

Total reflux is the condition when all the condensate is returned to the column as reflux: No product is taken off, and there is no feed.

At total reflux, the number of stages required for a given separation is the minimum at which it is theoretically possible to achieve the separation. Though not a practical operating condition, it is a useful guide to the likely number of stages that will be needed.

Columns are often started up with no product take-off and operated at total reflux until steady conditions are attained. The testing of columns is also conveniently carried out at total reflux.

Minimum reflux

As the reflux ratio is reduced, a *pinch point* will occur at which the separation can only be achieved with an infinite number of stages. This sets the minimum possible reflux ratio for the specified separation.

Optimum reflux ratio

Practical reflux ratios will lie somewhere between the minimum for the specified separation and total reflux. The designer must select a value at which the specified separation is achieved at minimum cost. Increasing the reflux reduces the number of stages required, and hence the capital cost, but increases the utility requirements (steam and cooling water) and the operating costs. The optimum reflux ratio will be that which gives the lowest total annualized cost or greatest net present value. No hard and fast rules can be given for the selection of the design reflux ratio, but for many systems the optimum will lie between 1.1 and 1.3 times the minimum reflux ratio. As a first approximation, 1.15 times minimum reflux is often used.

For new designs, where the ratio cannot be decided on from past experience, the effect of reflux ratio on the number of stages can be investigated using a process simulation model.

At low reflux ratios, the calculated number of stages will be highly dependent on the accuracy of the vapor–liquid equilibrium data available. If the data or phase equilibrium model is suspect, the designer should select a higher-than-normal ratio to give more confidence in the design.

17.2.2 Feed-point location

The precise location of the feed point will affect the number of stages required for a specified separation and the subsequent operation of the column. As a general rule, the feed should enter the column at the point that gives the best match between the feed composition (vapor and liquid if two phases) and the vapor and liquid streams in the column. In practice, it is wise to provide two or three feed-point nozzles located near the predicted feed point to allow for uncertainties in the design calculations and data and possible changes in the feed composition after start-up.

17.2.3 Selection of column pressure

Except when distilling heat-sensitive materials, the main consideration when selecting the column operating pressure will be to ensure that the dew point of the distillate is above the temperature that can be easily obtained with plant cooling water. The maximum, summer, temperature of cooling water is usually taken as 30 °C. If this means that high pressures will be needed, the provision of refrigerated cooling should be considered. Vacuum operation is used to reduce the column temperatures for the distillation of heat-sensitive materials and where very high temperatures would otherwise be needed to distil relatively nonvolatile materials.

When calculating the stage and reflux requirements using shortcut methods, it is usual to take the operating pressure as constant throughout the column. In vacuum columns, the column pressure drop will be a significant fraction of the total pressure, and the change in pressure up the column should be allowed for when calculating the stage temperatures. When using rigorous simulation methods, a rough initial estimate of column pressure drop can be made by assuming a pressure drop per tray equal to twice the liquid static head on the tray, that is, $2\,\rho_L\,g\,h_w$, where ρ_L is the liquid density (kg/m^3), g is the gravitational acceleration (m/s^2), and h_w is the weir height (m).

17.3 Continuous distillation: Basic principles

17.3.1 Stage equations

Material and energy balance equations can be written for any stage in a multistage process.

Fig. 17.2 shows the material flows into and out of a typical stage n in a distillation column. The equations for this stage are set out here, for any component i.

Material balance

$$V_{n+1}y_{n+1} + L_{n-1}x_{n-1} + F_n z_n = V_n y_n + L_n x_n + S_n x_n \tag{17.1}$$

Energy balance

$$V_{n+1}H_{n+1} + L_{n-1}h_{n-1} + Fh_f + q_n = V_n H_n + L_n h_n + S_n h_n \tag{17.2}$$

where V_n = vapor flow from the stage
V_{n+1} = vapor flow into the stage from the stage below
L_n = liquid flow from the stage
L_{n-1} = liquid flow into the stage from the stage above
F_n = any feed flow into the stage
S_n = any side stream from the stage
q_n = heat flow into, or removal from, the stage
n = any stage, numbered from the top of the column
z = mol fraction of component i in the feed stream (note, feed may be two-phase)
x = mol fraction of component i in the liquid streams
y = mol fraction component i in the vapor streams
H = specific enthalpy vapor phase
h = specific enthalpy liquid phase
h_f = specific enthalpy feed (vapor + liquid)

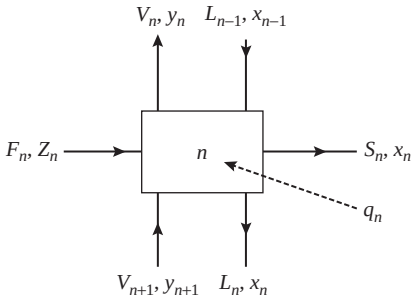


FIG. 17.2 Stage flows.

All flows are the total stream flows (mol/unit time), and the specific enthalpies are also for the total stream (J/mol).

It is convenient to carry out the analysis in terms of "equilibrium stages." In an equilibrium stage (theoretical plate), the liquid and vapor streams leaving the stage are taken to be in equilibrium, and their compositions are determined by the vapor–liquid equilibrium relationship for the system; see Chapter 4. In terms of equilibrium constants:

$$y_i = k_i x_i \tag{17.3}$$

The performance of real stages is related to an equilibrium stage by the concept of plate or stage efficiencies for plate contactors and "height equivalent to a theoretical plate" for packed columns.

In addition to the equations arising from the material and energy balances over a stage, and the equilibrium relationships, there will be a fourth relationship, the summation equation for the liquid and vapor compositions:

$$\Sigma x_{i,n} = \Sigma y_{i,n} = 1.0 \tag{17.4}$$

These four equations are the so-called MESH equations for the stage: Material balance, Equilibrium, Summation, and Heat (energy) balance equations. MESH equations can be written for each stage and for the reboiler and condenser. The solution of this set of equations forms the basis of the rigorous methods that have been developed for the analysis of staged separation processes and that are solved in the process simulation programs.

17.3.2 Dew point and bubble point

To estimate the stage, condenser, and reboiler temperatures, procedures are required for calculating dew and bubble points. By definition, a saturated liquid is at its bubble point (any rise in temperature will cause a bubble of vapor to form) and a saturated vapor is at its dew point (any drop in temperature will cause a drop of liquid to form).

Dew points and bubble points can be calculated from the vapor–liquid equilibrium for the system. In terms of equilibrium constants, the bubble point is defined by the equation:

$$\text{bubble point: } \Sigma y_i = \Sigma K_i x_i = 1.0 \tag{17.5a}$$

$$\text{and dew point: } \Sigma x_i = \Sigma \frac{y_i}{K_i} = 1.0 \tag{17.5b}$$

For multicomponent mixtures, the temperature that satisfies these equations, at a given system pressure, must be found by iteration. For binary systems, the equations can be solved more readily because the component compositions are not independent; fixing one fixes the other.

$$y_a = 1 - y_b \tag{17.6a}$$

$$x_a = 1 - x_b \tag{17.6b}$$

17.3.3 Equilibrium flash calculations

In an equilibrium flash process, a feed stream is separated into liquid and vapor streams at equilibrium. The composition of the streams depends on the quantity of the feed vaporized (flashed). The equations used for equilibrium flash calculations are developed later, and a typical calculation is shown in Example 17.1.

Flash calculations are often needed to determine the condition of the feed to a distillation column and, occasionally, to determine the flow of vapor from the reboiler, or condenser if a partial condenser is used.

Single-stage flash distillation processes are used to make a coarse separation of the light components in a feed, often as a preliminary step before a multicomponent distillation column.

Fig. 17.3 shows a typical equilibrium flash process. The equations describing this process are:

Material balance, for any component, i

$$F_{zi} = V_{yi} + L_{xi} \tag{17.7}$$

Energy balance, total stream enthalpies:

$$Fh_f = VH + Lh \tag{17.8}$$

If the vapor–liquid equilibrium relationship is expressed in terms of equilibrium constants, Equation 17.7 can be written in a more useful form:

$$\begin{aligned} Fz_i &= VK_i x_i + Lx_i \\ &= Lx_i \left[\frac{V}{L}K_i + 1\right] \end{aligned}$$

from which

$$L = \sum_i \frac{Fz_i}{\left[\dfrac{VK_i}{L} + 1\right]} \tag{17.9}$$

and, similarly,

$$V = \sum_i \frac{Fz_i}{\left[\dfrac{L}{VK_i + 1}\right]} \tag{17.10}$$

The groups incorporating the liquid and vapor flow rates and the equilibrium constants have a general significance in separation process calculations.

The group L/VK_i is known as the absorption factor, A_i, and is the ratio of the moles of any component in the liquid stream to the moles in the vapor stream.

The group VK_i/L is called the stripping factor, S_i, and is the reciprocal of the absorption factor.

Efficient techniques for the solution of the trial and error calculations necessary in multicomponent flash calculations are given by several authors, including Hengstebeck (1976) and King (1980). Flash models are available in all the commercial process simulation programs and are easy to configure. It is often a good idea to use flash models to check that the phase equilibrium model that has been selected makes an accurate prediction of any experimental data that are available. Flash models are also useful for checking for changes in volatility order or formation of second liquid phases within a distillation column.

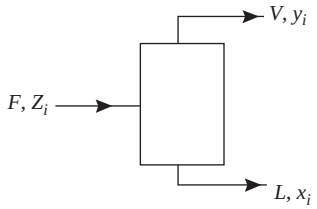


FIG. 17.3 Flash distillation.

Example 17.1

A feed to a column has the composition given in the following table and is at a pressure of 14 bar and a temperature of 60 °C. Calculate the flow and composition of the liquid and vapor phases. Equilibrium data can be taken from De Priester charts (Dadyburjor, 1978).

	kmol/h	z_i
Feed ethane (C_2)	20	0.25
propane (C_3)	20	0.25
isobutane (iC_4)	20	0.25
n-pentane (nC_5)	20	0.25

Solution

For two phases to exist, the flash temperature must lie between the bubble point and dew point of the mixture.
From Equations 17.5a and 17.5b:

$$\sum K_i z_i > 1.0$$

$$\Sigma \frac{z_i}{K_i} > 1.0$$

Check the feed condition:

	K_i	$K_i z_i$	z_i/K_i
C_2	3.8	0.95	0.07
C_3	1.3	0.33	0.19
iC_4	0.43	0.11	0.58
nC_5	0.16	0.04	1.56
		Σ 1.43	Σ 2.40

Therefore the feed is a two-phase mixture.
Flash calculation:

		Try $L/V = 1.5$		Try $L/V = 3.0$	
	K_i	$A_i = L/VK_i$	$V_i = Fz_i/(1 + A_i)$	A_i	V_i
C_2	3.8	0.395	14.34	0.789	11.17
C_3	1.3	1.154	9.29	2.308	6.04
iC_4	0.43	3.488	4.46	6.977	2.51
nC_5	0.16	9.375	1.93	18.750	1.01
		$V_{calc} = 30.02$		$V_{calc} = 20.73$	
		$L/V = \frac{80-30.02}{30.02} = 1.67$		$L/V = 2.80$	

Hengstebeck's method is used to find the third trial value for L/V. The calculated values are plotted against the assumed values, and the intercept with a line at 45 degrees (calculated = assumed) gives the new trial value: 2.4.

	Try $L/V = 2.4$			
	A_i	V_i	$y_i = V_i/V$	$x_i = (Fz_i - V_i)/L$
C_2	0.632	12.26	0.52	0.14
C_3	1.846	7.03	0.30	0.23
iC_4	5.581	3.04	0.13	0.30
nC_5	15.00	1.25	0.05	0.33
	$V_{cal} = 23.58$		1.00	1.00

$L = 80 - 23.58 = 56.42$ kmol/h

L/V calculated $= 56.42/23.58 = 2.39$ close enough to the assumed value of 2.4

Adiabatic flash

In many flash processes the feed stream is at a higher pressure than the flash pressure and the heat for vaporization is provided by the enthalpy of the feed. In this situation the flash temperature will not be known and must be found by iteration. A temperature must be found at which both the material and energy balances are satisfied. This is easily solved using process simulation software by specifying the flash outlet pressure and specifying zero heat input. The program then calculates the temperature and stream flow rates that satisfy the MESH equations.

17.4 Design variables in distillation

It was shown in Chapter 1 that to carry out a design calculation, the designer must specify values for a certain number of independent variables to define the problem completely and that the ease of calculation will often depend on the judicious choice of these design variables. The choice of design variables is particularly important in distillation, as the problem must be sufficiently well defined to find a feasible solution when simulated using a computer.

The total number of variables and equations required to describe a multicomponent distillation can be very large, because the MESH equations must be solved for every stage, including the reboiler and condenser. It becomes difficult for the designer to keep track of all the variables and equations, and mistakes are likely to be made, as the number of degrees of freedom will be the difference between two large numbers. Instead, a simpler procedure known as the "description rule" given by Hanson et al. (1962) can be used. The description rule states that to determine a separation process completely, the number of independent variables that must be set (by the designer) will equal the number that are set in the construction of the column or that can be controlled by external means in its operation. The method is best illustrated by considering the operation of the simplest type of column: with one feed, no side streams, a total condenser, and a reboiler. The construction will fix the number of stages above and below the feed point (two variables). The feed rate, column pressure, and condenser and reboiler duties (cooling water and steam flows) will be controlled (four variables). There are therefore six variables in total.

To design the column this number of variables must be specified, but the same variables need not be selected. Typically, in a design situation the feed rate will be fixed by the upstream design. The column pressure will also usually be fixed early in the design. Distillation processes are usually operated at low pressure, where relative volatility is high, but the pressure is usually constrained to be high enough for the condenser to operate using cooling water rather than refrigeration. If the feed rate and pressure are specified, then four degrees of freedom remain. Rigorous column models in process simulation programs require the designer to specify the number of stages above and below the feed, leaving the designer with two degrees of freedom. If two additional independent parameters are specified, then the problem is completely defined and has a single solution. For example, if the designer specifies a reflux ratio and a boil-up ratio or a reflux ratio and a distillate rate, then there will be a corresponding unique set of distillate and bottoms compositions for a given feed composition. If the designer chooses to specify the compositions of two key components in either the distillate or the bottoms, then there will be a required reflux rate, boil-up rate, distillate flow rate, etc. Similarly, specifying the purity and recovery of a single component in one of the products will completely specify the problem.

When replacing variables identified by the application of the description rule, it is important to ensure that those selected are truly independent and that the values assigned to them lie within the range of possible, practical values. For example, if the distillate mass flow rate is specified, then the bottoms flow rate is fixed by overall material balance and cannot be specified independently. Proper attention to the specification of variables is particularly important when using purity or composition specifications in multicomponent distillation. It would clearly not be possible to obtain 99% purity of the light key component in the distillate if the feed contained 2% of components that boiled at lower temperatures than the light key component. The selection of key components and product specifications for multicomponent distillation are discussed in more detail in Section 17.6.

The number of independent variables that have to be specified to define a problem will depend on the type of separation process being considered. Some examples of the application of the description rule to more complex columns are given by Hanson et al. (1962).

17.5 Design methods for binary systems

The distillation of binary mixtures is a relatively simple problem. With a binary mixture, fixing the composition of one component fixes the composition of the other. The stage and reflux requirements can be determined using simple graphical methods developed in the 1920s, and iterative calculations are not required.

It must be emphasized, however, that the graphical methods for binary distillation are no longer used in any practical context. Very few industrial distillation problems involve true binary mixtures. Other components will usually be present even if the two main components constitute more than 99.9 mol% of the mixture. The design engineer will usually need to know how these other components distribute between the distillate and bottoms to ensure that product specifications can be met and to determine the contaminant loads on downstream operations. Furthermore, the distillation design problem is seldom solved in isolation from the overall process design, and the widespread use of process simulation programs has made the graphical methods obsolete. The initialization of a rigorous simulation of a binary distillation uses the same methods used for a multicomponent distillation described in Section 4.5.2. The graphical methods give no insight into the solution procedures used for multicomponent distillation.

Despite these considerations, many educators find the graphical methods for binary distillation to be useful as a means of explaining some of the phenomena that can occur in multistage separations, and these methods are part of the required chemical engineering curriculum in most countries. The graphical methods can be used to illustrate some problems that are common to binary and multicomponent distillation. Graphical methods are still useful in understanding and initializing other staged separation processes such as absorption, stripping, and extraction.

The discussion of binary distillation methods in this chapter has been limited to a brief overview with emphasis on the insights that can be obtained from the graphs. For more details of the classical binary distillation methods, see Chhabra and Gurappa (2019) and earlier editions of this book.

17.5.1 Basic equations

Sorel (1899) first derived and applied the basic stage equations to the analysis of binary systems. Fig. 17.4(a) shows the flows and compositions in the top part of a column. Taking the system boundary to include the stage n and the condenser gives the following equations:

Material balance

total flows

$$V_{n+1} = L_n + D \tag{17.11}$$

where D is the distillate flow rate, and for either component:

$$V_{n+1}y_{n+1} = L_n x_n + Dx_d \tag{17.12}$$

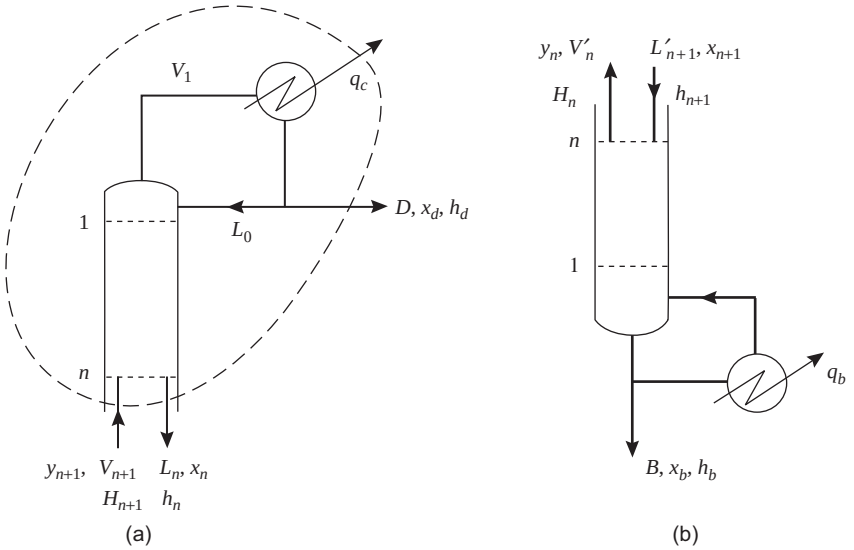


FIG. 17.4 Column flows and compositions. (a) Above feed. (b) Below feed.

Energy balance

total stream enthalpies

$$V_{n+1}H_{n+1} = L_n h_n + Dh_d + q_c \tag{17.13}$$

where q_c is the heat removed in the condenser.

Combining Equations 17.11 and 17.12 gives

$$y_{n+1} = \frac{L_n}{L_n + D}\, x_n + \frac{D}{L_n + D}\, x_d \tag{17.14}$$

Combining Equations 17.11 and 17.13 gives

$$V_{n+1}H_{n+1} = (L_n + D)H_{n+1} = L_n h_n + Dh_d + q_c \tag{17.15}$$

Analogous equations can be written for the stripping section (Fig. 17.4b).

$$x_{n+1} = \frac{V'_n}{V'_n + B}\, y_n + \frac{B}{V'_n + B}\, x_b \tag{17.16}$$

and

$$L'_{n+1}h_{n+1} = (V'_n + B)h_{n+1} = V'_n H_n + Bh_b - q_b \tag{17.17}$$

where B is the bottoms flow rate.

At constant pressure, the stage temperatures will be functions of the vapor and liquid compositions only (dew and bubble points), and the specific enthalpies will therefore also be functions of composition

$$H = \mathrm{f}(y) \tag{17.18a}$$

$$h = \mathrm{f}(x) \tag{17.18b}$$

Lewis–Sorel method (equimolar overflow)

For most distillation problems a simplifying assumption, first proposed by Lewis (1909), can be made that eliminates the need to solve the stage energy-balance equations. The molar liquid and vapor flow rates are taken as constant in the stripping and rectifying sections. This condition is referred to as equimolar overflow: the molar vapor and liquid flows from each stage are constant. This will only be true where the component molar latent heats of vaporization are the same and, together with the specific heats, are constant over the range of temperature in the column; there is no significant heat of mixing; and the heat losses are negligible. These conditions are substantially true for practical systems when the components form near-ideal liquid mixtures.

Even when the latent heats are substantially different, the error introduced by assuming equimolar overflow to calculate the number of stages is often small compared with the error in the stage efficiency and is acceptable.

With equimolar overflow, Equations 17.14 and 17.16 can be written without the subscripts to denote the stage number:

$$y_{n+1} = \frac{L}{L + D}\, x_n + \frac{D}{L + D}\, x_d \tag{17.19}$$

$$x_{n+1} = \frac{V'}{V' + B}\, y_n + \frac{B}{V' + B}\, x_b \tag{17.20}$$

where L = the constant liquid flow in the rectifying section = the reflux flow, L_0, and V' is the constant vapor flow in the stripping section.

Equations 17.19 and 17.20 can be written in an alternative form:

$$y_{n+1} = \frac{L}{V}\, x_n + \frac{D}{V}\, x_d \tag{17.21}$$

$$y_n = \frac{L'}{V'}\, x_{n+1} - \frac{B}{V'}\, x_b \tag{17.22}$$

where V is the constant vapor flow in the rectifying section $= (L + D)$, and L' is the constant liquid flow in the stripping section $= V' + B$.

These equations are linear, with slopes L/V and L'/V'. They are referred to as *operating lines* and give the relationship between the liquid and vapor compositions between stages. For an equilibrium stage, the compositions of the liquid and vapor streams leaving the stage are given by the equilibrium relationship.

17.5.2 McCabe–Thiele method

Equations 17.21 and 17.22 and the equilibrium relationship are conveniently solved by the graphical method developed by McCabe and Thiele (1925). A simple procedure for the construction of the diagram is given next and illustrated in Example 17.2.

Procedure

Refer to Fig. 17.5; all compositions are those of the more volatile component.

1. Plot the vapor–liquid equilibrium curve from data available at the column operating pressure. In terms of relative volatility:

$$y = \frac{\alpha x}{(1 + (\alpha - 1)x)} \tag{17.23}$$

   where α is the geometric average relative volatility of the lighter (more volatile) component with respect to the heavier component (less volatile).
   It is usually more convenient, and less confusing, to use equal scales for the x- and y-axes.
2. Make a material balance over the column to determine the top and bottom compositions, x_d and x_b, from the data given.
3. The upper and lower operating lines intersect the diagonal at x_d and x_b, respectively; mark these points on the diagram.
4. The point of intersection of the two operating lines is dependent on the phase condition of the feed. The line on which the intersection occurs is called the *q line.* The q line is found as follows:
   i. Calculate the value of the ratio q given by

$$q = \frac{\text{heat to vaporize 1 mol of feed}}{\text{molar latent heat of feed}}$$

   ii. Plot the q line, slope $= q/(q - 1)$, intersecting the diagonal at z_f (the feed composition).

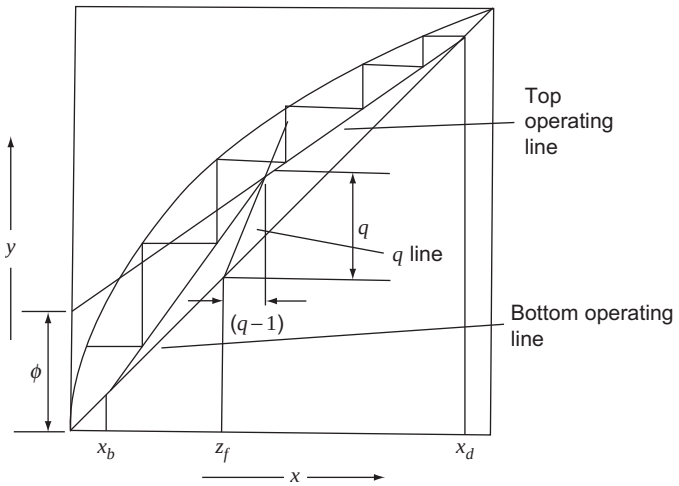


FIG. 17.5 McCabe–Thiele diagram.

5. Select the reflux ratio and determine the point where the upper operating line extended cuts the y-axis:

$$\phi = \frac{x_d}{1+R} \tag{17.24}$$

6. Draw in the upper operating line (UOL) from x_d on the diagonal to ϕ.
7. Draw in the lower operating line (LOL) from x_b on the diagonal to the point of intersection of the top operating line and the q line.
8. Starting at x_d or x_b, step off the number of stages.

Note: The feed point should be located on the stage closest to the intersection of the operating lines.

The reboiler, and a partial condenser if used, act as equilibrium stages; however, when designing a column there is little point in reducing the estimated number of stages to account for this. Not counting the reboiler as a stage can be considered an additional design margin.

It can be seen from Equation 17.24 and Fig. 17.5 that as R increases, ϕ decreases until the limit is reached where $\phi = 0$ and the upper and lower operating lines both lie along the diagonal, as in Fig. 17.6. This is the total reflux condition in which the minimum number of stages is needed for the separation.

Similarly, as R is reduced, the intersection between the upper and lower operating lines moves away from the diagonal until it reaches the equilibrium line, as illustrated in Fig. 17.7. This is the minimum reflux condition. If the reflux ratio were to be reduced further, then there would be no feasible intersection of the operating lines.

It can also be seen that at minimum reflux the space between the operating and equilibrium lines becomes very small at the intersection point, which is known as a "pinched" condition. An infinite number of trays is required at minimum reflux because of these pinch points, as can be seen in Fig. 17.7. Pinch points also often occur when the relative volatility of the mixture is not constant, particularly when azeotropes or near azeotropes form, as illustrated in Fig. 17.9. Pinch points also occur at the top or bottom of the column if very stringent purity specifications must be met.

Pinch points are also found in multicomponent distillation and are easily visualized as regions where the composition profiles appear to be varying only very slightly from stage to stage. When a pinch point occurs, the solution is usually to increase the reflux or change column pressure to obtain a more favorable equilibrium.

The efficiency of real contacting stages can be accounted for by reducing the height of the steps on the McCabe–Thiele diagram (Fig. 17.8). Stage efficiencies are discussed in Section 17.10.

The McCabe–Thiele method can be used for the design of columns with side streams and multiple feeds. The liquid and vapor flows in the sections between the feed and take-off points are calculated and operating lines drawn for each section.

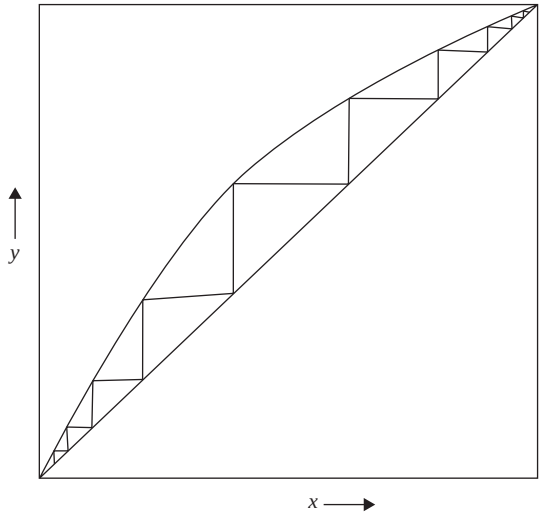


FIG. 17.6 Total reflux.

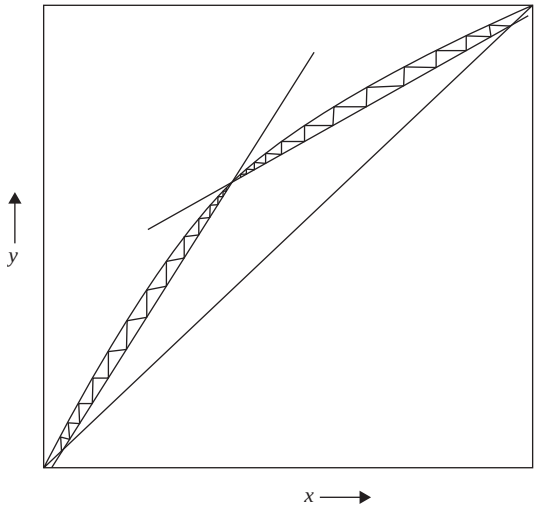


FIG. 17.7 Minimum reflux.

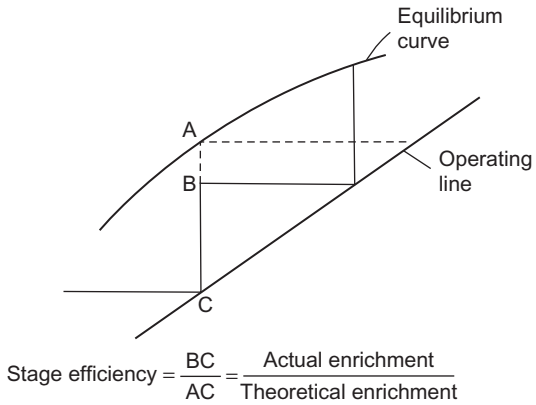


FIG. 17.8 Stage efficiency.

Example 17.2

Acetone is to be recovered from an aqueous waste stream by continuous distillation. The feed contains 10 mol% acetone. Acetone of at least 95 mol% purity is wanted, and the aqueous effluent must not contain more than 1 mol% acetone. The feed will be a saturated liquid. Estimate the number of ideal stages required.

Solution

There is no point in operating this column at other than atmospheric pressure. The equilibrium data of Kojima et al. (1968) will be used.

Mol fraction x, liquid	0.00	0.05	0.10	0.15	0.20	0.25	0.30
Acetone y, vapor	0.00	0.6381	0.7301	0.7716	0.7916	0.8034	0.8124
Bubble point °C	100.0	74.80	68.53	65.26	63.59	62.60	61.87
x	0.35	0.40	0.45	0.50	0.55	0.60	0.65
y	0.8201	0.8269	0.8376	0.8387	0.8455	0.8532	0.8615
°C	61.26	60.75	60.35	59.95	59.54	59.12	58.71
x	0.70	0.75	0.80	0.85	0.90	0.95	
y	0.8712	0.8817	0.8950	0.9118	0.9335	0.9627	
°C	58.29	57.90	57.49	57.08	56.68	56.30	

The equilibrium curve can be drawn with sufficient accuracy to determine the stages above the feed by plotting the concentrations at increments of 0.1.

Following the procedure given here, we can mark the product compositions.

Because the feed is a saturated liquid, $q = 1$, and the slope of the q line is $1/(1 - 1) = \infty$. The q line is thus plotted as a vertical line through the feed composition.

For this problem, the condition of minimum reflux occurs where the top operating line just touches the equilibrium curve at the point where the q line cuts the curve.

From Fig. 17.9,

$$\Phi \text{ for the operating line at minimum reflux} = 0.59$$

From Equation 17.24, $R_{\text{min}} = 0.95/0.59 - 1 = 0.62$

Take $R = R_{\text{min}} \times 2 = 1.24$

As the flows above the feed point will be small, a high reflux ratio is justified; the condenser duty will be small.

$$\varphi = \frac{0.95}{1 + 1.24} = 0.42$$

We can then plot the UOL and LOL.

Stepping off from the bottom, we require two stages in the stripping section and an additional eight stages in the rectifying section. The feed should be on the third stage from the bottom. Note that the number of stages below the feed is small, and because the reboiler counts as an equilibrium stage, if we feed onto the third plate from the bottom, we would actually be feeding onto the stage marked 4 in Fig. 17.9. This feed would be badly mismatched with the vapor and liquid compositions in the column, so it would be advisable to allow for possible feeds to the second and third plates from the bottom so that the feed point can be moved. Note also that the column is close to pinched at the top of the rectifying section. It would be prudent to add extra trays in this section.

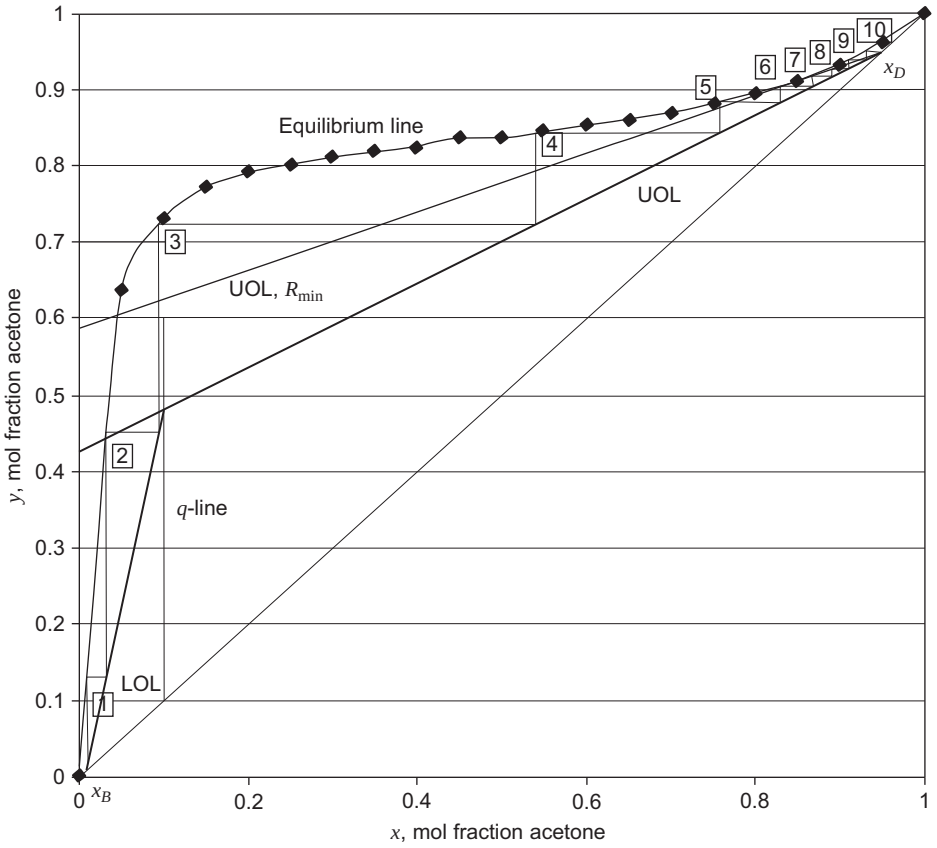


FIG. 17.9 McCabe–Thiele plot, Example 17.2.

17.6 Multicomponent distillation: General considerations

The problem of determining the stage and reflux requirements for multicomponent distillations is much more complex than for binary mixtures. With a multicomponent mixture, fixing one component composition does not uniquely determine the other component compositions and the stage temperature. Also when the feed contains more than two components, it is not possible to specify the complete composition of the top and bottom products independently. The separation between the top and bottom products is usually specified by setting limits on two "key" components, between which it is desired to make the separation.

The complexity of multicomponent distillation calculations can be appreciated by considering a typical problem. The normal procedure is to solve the MESH equations (Section 17.3.1), stage by stage, from the top or bottom of the column. For such a calculation to converge to a solution, the compositions obtained from either the bottom-up or top-down calculations must match the composition at the other end of the column predicted from an overall material balance. But the calculated compositions will depend on the compositions assumed for the top or bottom products at the start of the calculations. Though it is possible to match the key components, the other components will not match unless the designer was particularly fortunate in choosing the trial top and bottom compositions. For a completely rigorous solution, the compositions must be adjusted and the calculations repeated until satisfactory convergence is obtained. Clearly, the greater the number of components considered, the more difficult the problem. As was shown in Section 17.3.2, iterative calculations will be needed to determine the stage temperatures. For other than ideal mixtures, the calculations will be further complicated by the fact that the component volatilities will be functions of the unknown stage compositions and temperatures. The relationship between volatility, composition, and temperature may be highly nonlinear, as discussed in Chapter 4. If more than a few stages are required, stage-by-stage calculations are complex and tedious, and even with sophisticated process simulation programs convergence cannot be guaranteed.

Before the widespread availability of digital computers, various "shortcut" methods were developed to simplify the task of designing multicomponent columns. A comprehensive summary of the methods used for hydrocarbon systems is given by Edmister (1947 to 1949) in a series of articles in the journal *The Petroleum Engineer*. Though computer programs will normally be available for the rigorous solution of the MESH equations, shortcut methods are still useful in preliminary design work and as an aid in initializing problems for computer solution.

17.6.1 Key components

Before starting the column design, the designer must select the two *key* components between which it is desired to make the separation. The light key will be the component that it is desired to keep out of the bottom product, and the heavy key the component to be kept out of the top product. The keys are known as *adjacent keys* if they are "adjacent" in a listing of the components in order of volatility, and *split keys* or *nonadjacent keys* if some other component lies between them in the volatility order. A separation between adjacent keys is known as a *sharp split*, whereas a separation with nonadjacent keys is known as a *sloppy split*.

The choice of key components will normally be clear, but sometimes, particularly if close boiling isomers are present, judgment must be used in their selection. If any uncertainty exists, trial calculations should be made using different components as the keys to determine the pair that requires the largest number of stages for separation (the worst case). The Fenske equation can be used for these calculations; see Section 17.7.1.

The *nonkey* components that appear in both top and bottom products are known as *distributed* components; and those that are not present, to any significant extent, in one or other product, are known as *nondistributed* components.

17.6.2 Product specifications

Specifications for the column will normally be set in terms of the purity or recovery of the key components.

A purity specification sets the mole (or mass) fraction of a component in one of the product streams. Purity specifications are easily understood and are easy to relate to the required product specifications. For example, if the standard specification for the desired grade of product is 99.5% pure, then the designer could specify 99.5% purity of the product in the distillate of a finishing column. Similarly, if the purity of the heavy key component in the distillate must be less than 50 ppm, then this can be used as the specification.

Although purity specifications are intuitively obvious, their use often leads to infeasible column specifications. The designer must check carefully to ensure that the amounts of lighter-than-light-key (or heavier-than-heavy-key) components are not large enough to render the purity specification infeasible. Consider, for example, a feed that contains 0.5 mol% A, 49.5 mol% B, and 50 mol% C, where A is most volatile and C is least volatile. The highest purity of B that can be obtained in the distillate is 99%, and that would require complete recovery of B and complete rejection of C from the distillate, with a very high reflux ratio. If only 99% of the C is recovered in the bottoms product and only 99% of the B is recovered overhead, then the maximum feasible purity of B is $0.99(49.5)/[0.5 + 0.99(49.5) + 0.5] = 98\%$.

When a purity specification must be met in a column that forms part of a multicomponent sequence of columns, it is essential to set the specifications of the other columns so that the desired purity specification is feasible.

Instead of specifying purity, the designer can specify the recovery of one or more of the key components in either the distillate or bottoms. The recovery of a component in a product stream is defined as the fraction of the feed molar flow rate of the component that is recovered in that product stream. The relationship between purity and recovery is often not simple, particularly when many components are present or the key components are nonadjacent.

Recovery specifications are easily related to economic trade-offs, because the value of recovering an additional 0.1% or 0.01% of the desired product is easily assessed and can be traded off against the additional capital and operating costs of the column. Recovery of the desired product is usually set at 99% or greater. Recovery specifications for a distillation column are less likely to be infeasible than purity specifications; however, their use does not guarantee that the product will meet the specifications required for sale.

In general, it is better to use purity specifications for the final column that produces product (usually termed the *finishing column*) and recovery specifications elsewhere in the distillation sequence. A combination of purity and recovery specifications can also be used for a single column. For example, in a finishing column in which the desired product is taken as distillate, the designer could specify the purity and recovery of the desired (light key) component in the distillate. No specifications on the heavy key or other components are needed, but the same feasibility checks must be made for the purity specification.

In mixtures that form azeotropes, the volatility order changes with composition. This creates additional problems when setting product specifications. The design of azeotropic distillation sequences is discussed in Section 17.6.5.

Most process simulation programs allow the designer to select two specifications for a distillation column corresponding to the two remaining degrees of freedom once the feed rate, pressure, number of stages, and feed stage have been selected. If the column is to be designed to achieve a given purity or recovery, then it obviously makes sense to use this as a specification if the simulation program allows it, but the designer may need to provide an initial estimate of other parameters such as reflux ratio or distillate rate to ensure good convergence. Estimates of these parameters can be made using shortcut calculations or shortcut column models, as described in Section 17.7. The use of shortcut models to initialize a rigorous simulation model was discussed in Section 4.5.2 and illustrated in Example 4.3. Example 4.4 showed the effect of changing to a recovery specification in a rigorous solution of the same problem.

In some cases, the simulation program or model may not allow the use of purity or recovery specifications, in which case the designer must adjust other variables such as reflux rate, boil-up rate and distillate, or bottoms flow rate until the specifications are met.

17.6.3 Number and sequencing of columns

In multicomponent distillation the production of a pure product usually requires at least two distillation columns. A common arrangement is to remove all components lighter than the desired product in a first column, then separate the desired product from heavier components in a second column. This arrangement is illustrated in Fig. 17.10, and

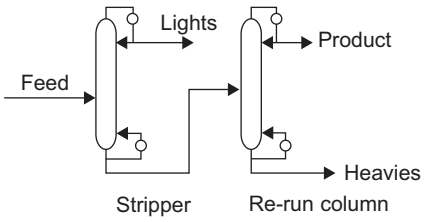


FIG. 17.10 Stripper and re-run column.

is known as a stripper and re-run column sequence. Because almost all processes produce some by-products that are lighter and some that are heavier than the desired product, this scheme is widely used.

If additional pure products are to be produced, additional columns will be needed. The recovery of an additional pure component from the lights stream in Fig. 17.10 would require one more column if the component were the least volatile component in the lights (i.e., the light key component of the first column in Fig. 17.10), or two more columns if there were any additional components that boiled between the two desired products.

If a mixture contained N components and the designer wanted to separate it into pure components, then $N - 1$ columns would be needed, as each component could be removed in order of volatility until the final binary pair remained. If only M pure products are required, then the number of columns needed is generally bounded between $M + 1$ and either $2M$ or $N - 1$, whichever is least. It might be expected that the minimum number of columns would be M, but the presence of small amounts of light or heavy components invariably requires the designer to use at least one extra column to enable the product purity specification to be achieved.

The distillation sequence in which the components are separated in order of decreasing volatility is known as a *direct sequence* and is shown in Fig. 17.11(a). There are many other possible distillation sequences. Fig. 17.11(b) shows an *indirect sequence* in which the heaviest component is removed first and the distillate is fed to the second column. Components are then removed in order from least volatile to most volatile. Fig. 17.11(c) shows a mixed sequence in which the first separation is between components in the middle of the volatility order.

With five components, there are 14 possible column configurations. As the number of components increases, the number of possible column sequences increases combinatorially. With 10 components there are nearly 5000 possible schemes. The optimum scheme will be the one that has the best overall economic performance.

Various methods have been proposed for screening alternative designs to determine the optimum sequence; see Doherty and Malone (2001), Smith (2016), and Kumar (1982). These methods usually use shortcut column models and approximate costing relationships, so it is often worthwhile to complete detailed designs for a few of the best candidate schemes identified. There can also be strong interactions between the column sequence and the associated heat integration that can influence the final scheme that is selected.

Although distillation column sequencing is an interesting research problem, in practice there are very few processes that make more than two or three pure products. The optimum sequence can often be determined using heuristic rules such as:

1. Remove corrosive components first to avoid using expensive metallurgy throughout the sequence.
2. Remove the heaviest component first if solids are present in the feed. The presence of solids requires the use of special plates that are designed to resist plugging and have very low-stage efficiency. It is best to get the solids out of the way as early as possible.
3. Split any components that cannot be condensed using cooling water from those that can be condensed early in the sequence. The lighter components can then be compressed to higher pressure, separated using absorption or adsorption, or separated in refrigerated columns. This rule avoids the use of refrigerated condensers, higher pressures, or partial condensers elsewhere in the sequence.
4. Postpone the most difficult separation, such as between close-boiling compounds, until late in the sequence. A difficult separation will require many stages and high reflux, and so the feed rate to that column should be made as low as possible so that the column handles less material.
5. Take the desired products as distillates whenever practical to avoid any flushing of dirt or debris into the desired product. The same rule also applies to recycle streams.
6. Remove any components that are present in large excess early in the sequence to make the downstream columns cheaper.

Tall columns

Where a large number of stages is required, it may be necessary to split a column into two separate columns to reduce the height of the column, even though the required separation could, theoretically, have been obtained in a single column. This may also be done in vacuum distillations to reduce the column pressure drop and limit the bottom temperatures.

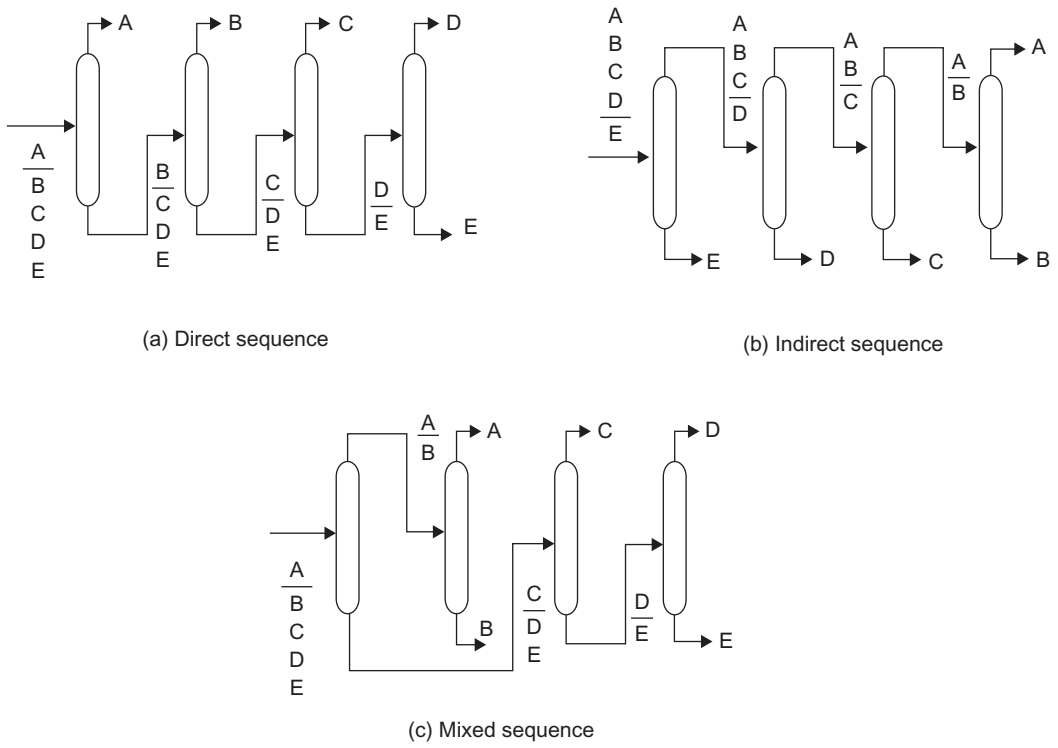


FIG. 17.11 Column sequences for a five-component mixture.

17.6.4 Complex columns

It is relatively easy to withdraw side streams from plate columns and to supply additional feeds to the column. If a liquid side stream is withdrawn from a tray above the feed, as shown in Fig. 17.12(a), it will be depleted in the heavier components of the feed (which preferentially stayed in the liquid phase and went down in the stripping section) and will also be depleted in the lighter components of the feed (which are preferentially in the vapor phase). Although the side stream will not be pure, it will be enriched in some of the components of midrange volatility. In some cases, the purity of the side stream may be adequate, for example, if the side stream is a process recycle.

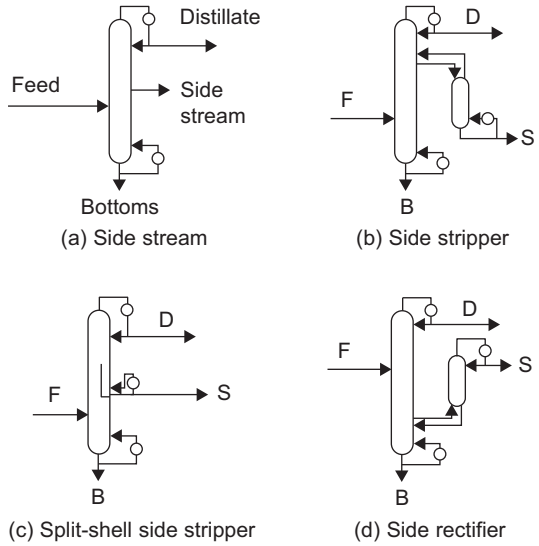
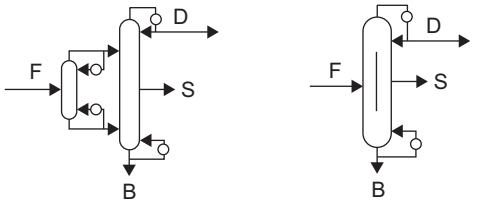


FIG. 17.12 Side streams and side columns.



(a) Prefractionator (b) Dividing wall column

FIG. 17.13 Complex column designs.

The purity of a desired component in the side stream can be increased by sending the side stream to a small side stripper column that strips out any lighter components, as shown in Fig. 17.12(b). The vapor from the side stripper is returned to the main column. A side stripper can be constructed as part of the maim column by using a partitioned section of the main column, as shown in Fig. 17.12(c). Side rectifiers are also used; see Fig. 17.12(d).

Side strippers and rectifiers allow up to three pure products to be made in one and a half columns, or in a single shell if a partition wall is used. Other complex column configurations are also possible, such as prefractionators and dividing wall columns, illustrated in Fig. 17.13. These complex columns generally have lower capital and operating costs than sequences of simple columns. More degrees of freedom are introduced into the design, so more care is needed in optimizing the columns. Smith (2016) gives an excellent introduction to the design of complex columns. Greene (2001), Schultz et al. (2002), Kaibel (2002), and Parkinson (2007) describe industrial applications of dividing wall columns. Side strippers are widely used in petroleum refining; see Watkins (1979). Most process simulators allow the designer to add side strippers and rectifiers or select from a set of prebuilt complex column models.

17.6.5 Distillation column sequencing for azeotropic mixtures

When a mixture forms an azeotrope, determining the best column sequence is not straightforward. Homogeneous azeotropes are mixtures of two or more components that have the same vapor- and liquid-phase composition at the boiling point. Heterogeneous azeotropes have two liquid phases that are in equilibrium with a vapor that has the same composition as the combined liquid composition at the boiling point. Different strategies are used for separation depending on the type of azeotrope.

The design of azeotropic distillation sequences has been the subject of much academic research, and there is not sufficient space here to describe all of the techniques that have been developed. The reader should refer to Smith (2016) and Doherty and Malone (2001) for a more detailed treatment of the subject. The general strategy for separating an azeotropic mixture can be summarized as:

1. If the azeotrope is heterogeneous, use a liquid−liquid split (decanter). The two liquid phases will usually have compositions on either side of the azeotrope. Each of these liquids can be distilled to give a pure product and the azeotrope, and the azeotropic mixtures can be recycled to the decanter. In some cases a third component, known as an entrainer, is added to cause the formation of a heterogeneous azeotropic mixture. The degree of separation in the liquid−liquid split can often be increased by lowering the temperature, which tends to increase the size of the two-phase region in the composition space.
   For example, Fig. 17.14 shows the separation of an ethanol−water mixture using benzene as entrainer. The ethanol−water mixture is distilled to give a low-boiling azeotrope, which is then sent to a first column that is refluxed with the oil phase from a decanter. The first column produces ethanol as bottom product and a heterogeneous azeotrope as distillate. The distillate is sent to a decanter and separated into oil-rich and water-rich phases. The water phase is sent to a second column that produces water as bottoms product and heterogeneous azeotrope as distillate. The distillate from the second column is also sent to the decanter. This flow scheme was widely used for ethanol dehydration until cheaper and safer processes based on adsorbing the water using molecular sieves were introduced.
   This flow scheme is sometimes known as *azeotropic distillation*; however, the term *heterogeneous azeotropic distillation* is better, as all of the other methods also involve distilling azeotropes.
2. If the azeotrope is homogeneous, then the effect of varying pressure should be investigated. The composition of the azeotrope is always pressure dependent. If there is a large change in composition over a reasonable range of pressure, two columns at different pressures can be used. Each column produces a pure product and a mixture corresponding to the azeotrope at the pressure of that column. The azeotropic mixture is then fed to the other

column, as illustrated in Fig. 17.15. The mixture from the low-pressure column must be pumped back up to the pressure of the high-pressure column. Note that the feed can be to either column and that it is also possible to produce the products as distillates if the azeotrope is maximum-boiling rather than minimum-boiling.
The pressure-swing distillation flow scheme is relatively simple and does not require any additional components to be added, but if the azeotrope composition is only weakly sensitive to pressure, the recycle from the low-pressure column to the high-pressure column will be large. The recycled material must be vaporized in the low-pressure column, so the low-pressure column can become quite expensive.

3. If pressure-swing distillation is not economically attractive, consider adding an entrainer. The preferred entrainers are usually those that form heterogeneous azeotropes, as discussed earlier, but homogeneous entrainers can also be used, in which case the process is known as extractive distillation.
The most commonly used type of entrainer is a higher boiling compound that does not form an azeotrope with either component of the azeotropic pair. If a high-boiling entrainer is used, it depresses the volatility of one component of the azeotrope, allowing the other component to be recovered in the distillate. The bottoms from the first column are then sent to a second column in which the other pure component is recovered as distillate and the entrainer is recovered as bottoms for recycle to the first column, as shown in Fig. 17.16. Other schemes with low-boiling or mid-boiling entrainers are also possible, as described by Doherty and Malone (2001).
The entrainer should be selected from compounds that are already present within the process whenever possible. The use of compounds that are already present reduces consumables costs and waste formation and usually makes it easier to reach product specifications. The other compounds that are present in the process can be screened for suitability as entrainers by looking at boiling points and checking for the formation of additional azeotropes. If nothing suitable is found, the more sophisticated methods for evaluating entrainers described by Doherty and Malone (2001) should be used.
4. If the azeotropic composition is close to the required purity specification, consider removing the minor component by adsorption using a selective sorbent. If a regenerable sorbent can be found, this process may be cheaper than a multicolumn distillation. Pressure-swing adsorption using a molecular sieve sorbent as drying agent is now the most widely used method for breaking the ethanol–water azeotrope. Adsorption processes are discussed in Chapter 16.
5. If a suitable membrane material can be found that is permeable to one component of the mixture but impermeable to the other, then membrane separation can be used in combination with distillation. A typical flowsheet for the case where the light component is permeable is shown in Fig. 17.17. A distillation column is used to separate the mixture of A and B into pure heavy component B and azeotrope. The azeotropic mixture is sent to the membrane unit, where pure light component A is recovered. It is usually not economical to operate a membrane unit at high recovery of permeate, so the retentate still contains a significant fraction of A and is recycled to the distillation column. If the membrane is not impermeable to component B, a permeate stream that is enriched in A can be sent to a second distillation column that then produces pure A and an azeotropic mixture for recycle to the membrane unit. The design of membrane processes is described in Chapter 16.

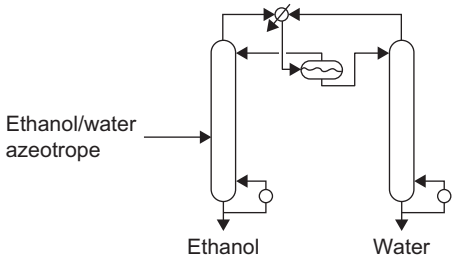


FIG. 17.14 Dehydration of ethanol using benzene as entrainer.

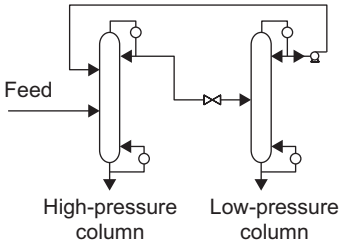


FIG. 17.15 Pressure-swing distillation.

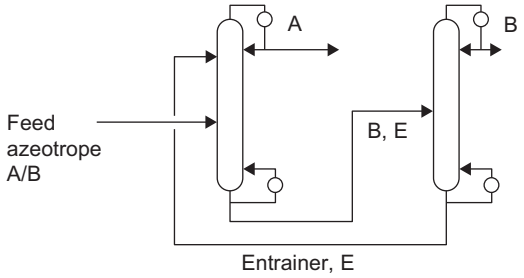


FIG. 17.16 Extractive distillation.

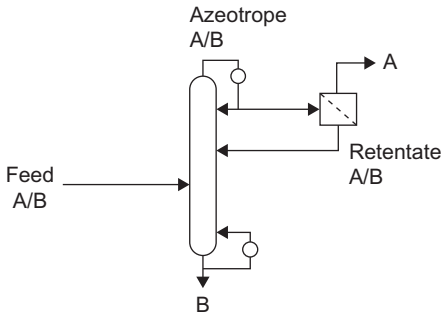


FIG. 17.17 Membrane distillation.

17.7 Multicomponent distillation: Shortcut methods for stage and reflux requirements

Some of the more useful shortcut procedures that can be used to estimate stage and reflux requirements without the aid of computers are given in this section. Most of the shortcut methods were developed for the design of separation columns for hydrocarbon systems in the petroleum and petrochemical industries, and caution must be exercised when applying them to other systems. They usually depend on the assumption of constant relative volatility and should not be used for severely nonideal systems. Shortcut methods for nonideal and azeotropic systems are given by Featherstone (1971, 1973).

Although the shortcut methods were developed for hand calculations, they are easily coded into spreadsheets and are available as subroutines in all the commercial process simulation programs. The shortcut methods are useful when configuring rigorous distillation models, as described in Section 4.5.2.

The two most frequently used empirical methods for estimating the stage requirements for multicomponent distillations are the correlations published by Gilliland (1940) and by Erbar and Maddox (1961). These relate the number of ideal stages required for a given separation, at a given reflux ratio, to the number at total reflux (minimum possible) and the minimum reflux ratio (infinite number of stages). The Erbar–Maddox correlation is given in this section, as it is now generally considered to give more reliable predictions than Gilliland's correlation. The Erbar–Maddox correlation is shown in Fig. 17.18, which gives the ratio of number of stages required to the number at total reflux, as a function of the reflux ratio, with the minimum reflux ratio as a parameter. To use Fig. 17.18, estimates of the number of stages at total reflux and the minimum reflux ratio are needed.

17.7.1 Minimum number of stages (Fenske equation)

The Fenske equation (Fenske, 1932) can be used to estimate the minimum stages required at total reflux. The derivation of this equation for a binary system is given in Chhabra and Gurappa (2019). The equation applies equally to multicomponent systems and can be written as:

$$\left[\frac{x_i}{x_r}\right]_d = \alpha_i^{N_{\min}} \left[\frac{x_i}{x_r}\right]_b \tag{17.25}$$

where $[x_i/x_r]$ = the ratio of the concentration of any component i to the concentration of a reference component r, and the suffixes d and b denote the distillate (d) and the bottoms (b)

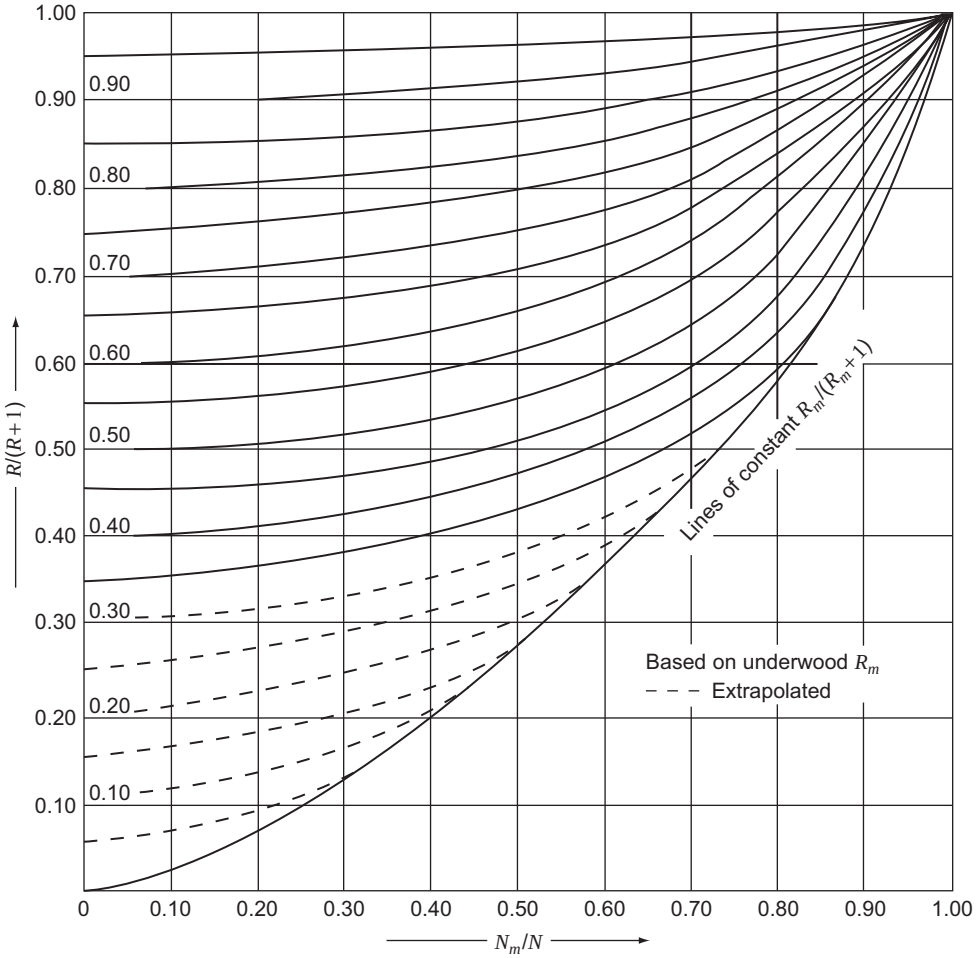


FIG. 17.18 Erbar–Maddox correlation. *(From Erbar & Maddox, 1961.)*

N_{min} = minimum number of stages at total reflux, including the reboiler
$_{\alpha i}$ = average relative volatility of the component i with respect to the reference component

Normally the separation required will be specified in terms of the key components, and Equation 17.25 can be rearranged to give an estimate of the number of stages.

$$N_{\min} = \frac{\log \left[\frac{x_{\mathrm{LK}}}{x_{\mathrm{HK}}}\right]_d \left[\frac{x_{\mathrm{HK}}}{x_{\mathrm{LK}}}\right]_b}{\log\ \alpha_{\mathrm{LK}}} \tag{17.26}$$

where $_{\alpha}$LK is the average relative volatility of the light key with respect to the heavy key, and x_{LK} and x_{HK} are the light and heavy key concentrations. The relative volatility is taken as the geometric mean of the values at the column top and bottom temperatures. To calculate these temperatures, initial estimates of the compositions must be made, so the calculation of the minimum number of stages by the Fenske equation is a trial-and-error procedure. The procedure is illustrated in Example 17.3. If there is a wide difference between the relative volatilities at the top and bottom of the column, the use of the average value in the Fenske equation will underestimate the number of stages. In these circumstances, a better estimate can be made by calculating the number of stages in the rectifying and stripping sections separately; taking the feed concentration as the base concentration for the rectifying section and as the top concentration for the stripping section, and estimating the average relative volatilities separately for each section. This procedure will also give an estimate of the feed point location.

Winn (1958) has derived an equation for estimating the number of stages at total reflux, which is similar to the Fenske equation, but which can be used when the relative volatility cannot be taken as constant.

If the number of stages is known, Equation 17.25 can be used to estimate the split of components between the top and bottom of the column at total reflux. It can be written in a more convenient form for calculating the split of components:

$$\frac{d_i}{b_i} = \alpha_i^{N_{\min}} \left[\frac{d_r}{b_r}\right] \tag{17.27}$$

where d_i and b_i are the flow rates of the component i in the distillate and bottoms and d_r and b_r are the flow rates of the reference component in the distillate and bottoms.

Note: From the column material balance:

$$d_i + b_i = f_i$$

where f_i is the flow rate of component i in the feed.

17.7.2 Minimum reflux ratio

Colburn (1941) and Underwood (1948) have derived equations for estimating the minimum reflux ratio for multicomponent distillations. As the Underwood equation is more widely used, it is presented in this section. The equation can be stated in the form:

$$\sum \frac{\alpha_i x_{i,d}}{\alpha_i - \theta} = R_{\min} + 1 \tag{17.28}$$

where α_i = the relative volatility of component i with respect to some reference component, usually the heavy key
R_{min} = the minimum reflux ratio
$x_{i,d}$ = concentration of component i in the distillate at minimum reflux
θ = the root of the equation:

$$\Sigma \frac{\alpha_i x_{i,f}}{\alpha_i - \theta} = 1 - q \tag{17.29}$$

where $x_{i,f}$ = the concentration of component i in the feed, and q depends on the condition of the feed and was defined in Section 17.5.2.

The value of θ must lie between the values of the relative volatility of the light and heavy keys and is found by trial and error.

In the derivation of Equations 17.28 and 17.29, the relative volatilities are taken as constant. The geometric average of values estimated at the top and bottom temperatures should be used. This requires an estimate of the top and bottom compositions. Though the compositions should strictly be those at minimum reflux, the values determined at total reflux, from the Fenske equation, can be used. A better estimate can be obtained by replacing the number of stages at total reflux in Equation 17.27 by an estimate of the actual number; a value equal to $N_{min}/0.6$ is often used. The Erbar–Maddox method of estimating the stage and reflux requirements, using the Fenske and Underwood equations, is illustrated in Example 17.3.

17.7.3 Feed-point location

A limitation of the Erbar–Maddox and similar empirical methods is that they do not give the feed-point location. An estimate can be made by using the Fenske equation to calculate the number of stages in the rectifying and stripping sections separately, but this requires an estimate of the feed-point temperature. An alternative approach is to use the empirical equation given by Kirkbride (1944):

$$\log\left[\frac{N_r}{N_s}\right] = 0.206 \log\left[\left(\frac{B}{D}\right)\left(\frac{x_{f,\mathrm{HK}}}{x_{f,\mathrm{LK}}}\right)\left(\frac{x_{b,\mathrm{LK}}}{x_{d,\mathrm{HK}}}\right)^2\right] \tag{17.30}$$

where N_r = number of stages above the feed, including any partial condenser
N_s = number of stages below the feed, including the reboiler
$x_{f,\mathrm{HK}}$ = concentration of the heavy key in the feed
$x_{f,\mathrm{LK}}$ = concentration of the light key in the feed
$x_{d,\mathrm{HK}}$ = concentration of the heavy key in the top product
$x_{b,\mathrm{LK}}$ = concentration of the light key if in the bottom product

The use of this equation is illustrated in Example 17.4.

Example 17.3

Estimate the minimum number of ideal stages needed in the butane–pentane splitter defined by the compositions given in the following table. The column will operate at a pressure of 8.3 bar. Evaluate the effect of changes in reflux ratio on the number of stages required. This is an example of the application of the Erbar–Maddox method. The feed is at its boiling point.

		Feed (f)	Distillate (d)	Bottoms (b)
Propane, C_3	5	5	0	
i-Butane, iC_4	15	15	0	
n-Butane, nC_4	25	24	1	
i-Pentane, iC_5	20	1	19	
n-Pentane, nC_5	35	0	35	
		100	45	55 kmol

Solution

The top and bottom temperatures (dew points and bubble points) were calculated by the method given in Section 17.3.2. Relative volatilities are given by:

$$\alpha_i = \frac{K_i}{K_{HK}}$$

Equilibrium constants were taken from De Priester charts (Dadyburjor, 1978).
Relative volatilities

	Top	Bottom	Average
Temp. °C	65	120	
C_3	5.5	4.5	5.0
iC_4	2.7	2.5	2.6
(LK) nC_4	2.1	2.0	2.0
(HK) iC_5	1.0	1.0	1.0
nC_5	0.84	0.85	0.85

Minimum number of stages; Fenske equation, Equation 17.26:

$$N_{min} = \frac{\log\left[\frac{24}{1}\right]\left[\frac{19}{1}\right]}{\log\ 2} = \underline{\underline{8.8}}$$

Minimum reflux ratio; Underwood Equations 17.28 and 17.29.
This calculation is best tabulated.
As the feed is at its boiling point q = 1:

$$\Sigma \frac{\alpha_i x_{i,f}}{\alpha_i - \theta} = 0 \qquad (17.29)$$

Try

$x_{i,f}$	α_i	$\alpha_i x_{i,f}$	$\theta = 1.5$	$\theta = 1.3$	$\theta = 1.35$
0.05	5	0.25	0.071	0.068	0.068
0.15	2.6	0.39	0.355	0.300	0.312
0.25	2.0	0.50	1.000	0.714	0.769
0.20	1	0.20	−0.400	−0.667	−0.571
0.35	0.85	0.30	−0.462	−0.667	−0.600
			$\Sigma = 0.564$	−0.252	0.022
					close enough

$\theta = 1.35$
Equation 17.28:

$x_{i,d}$	α_i	$\alpha_i x_{i,d}$	$\alpha_i x_{i,d}/(\alpha_i - \theta)$
0.11	5	0.55	0.15
0.33	2.6	0.86	0.69
0.53	2.0	1.08	1.66

$x_{i,d}$	α_i	$\alpha_i x_{i,d}$	$\alpha_i x_{i,d}/(\alpha_i - \theta)$
0.02	1	0.02	−0.06
0.01	0.85	0.01	−0.02
			$\Sigma = 2.42$

$$R_m + 1 = 2.42$$

$$R_m = \underline{\underline{1.42}}$$

$$\frac{R_m}{(R_m+1)} = \frac{1.42}{2.42} = 0.59$$

Specimen calculation for $R = 2.0$:

$$\frac{R}{(R+1)} = \frac{2}{3} = 0.66$$

From Fig. 17.18:

$$\frac{N_{\min}}{N} = 0.56$$

$$N = \frac{8.8}{0.56} = \underline{\underline{15.7}}$$

For other reflux ratios:

R	2	3	4	5	6
N	15.7	11.9	10.7	10.4	10.1

Note: The number of stages should be rounded up to the nearest integer. Above a reflux ratio of 4 there is little change in the number of stages required, but given the low number of theoretical stages needed, the optimum reflux ratio is probably less than 2.0.

Example 17.4

Estimate the position of the feed point for the separation considered in Example 17.3 for a reflux ratio of 3.

Solution

Use the Kirkbride equation, Equation 17.30. Product distributions are taken from Example 17.3, though they could be confirmed using Equation 17.27:

$$x_{b,\mathrm{LK}} = \frac{1}{55} = 0.018$$

$$x_{d,\mathrm{HK}} = \frac{1}{45} = 0.022$$

$$\log\left(\frac{N_r}{N_s}\right) = 0.206 \log\left[\frac{55}{45}\left(\frac{0.2}{0.25}\right)\left(\frac{0.018}{0.022}\right)^2\right]$$

$$\log\left(\frac{N_r}{N_s}\right) = 0.206 \log(0.65)$$

$$\left(\frac{N_r}{N_s}\right) = \underline{\underline{0.91}}$$

For $R = 3$, $N = 12$

Number of stages, excluding the reboiler = 11 :

$$N_r + N_s = 11$$

$$N_s = 11 - N_r = 11 - 0.91N_s$$

$$N_s = \frac{11}{1.91} = 5.76, \text{ say } 6$$

17.8 Multicomponent distillation: Rigorous solution procedures (computer methods)

The rigorous column models in the commercial process simulation programs solve the full set of MESH equations (Section 17.3.1). A considerable amount of work has been done to develop efficient and reliable computer-aided design procedures for distillation and other staged processes. A detailed discussion of this work is beyond the scope of this book, and the reader is referred to the specialist books that have been published on the subject: Smith (1963), Holland (1997), and Kister (1992), and to the numerous papers that have appeared in the chemical engineering literature. A good summary of the present state of the art is given by Haas (1992). In this section only a brief outline of the methods that have been developed will be given.

The basic steps in any rigorous solution procedure will be:

1. Specification of the problem; complete specification is essential for computer methods.
2. Selection of values for the iteration variables; for example, estimated stage temperatures and liquid and vapor flows (the column temperature and flow profiles).
3. A calculation procedure for the solution of the stage equations.
4. A procedure for the selection of new values for the iteration variables for each set of trial calculations.
5. A procedure to test for convergence; to check if a satisfactory solution has been achieved.

Rating and design methods

All the methods described here require the specification of the number of stages below and above the feed point. They are therefore not directly applicable to design: where the designer wants to determine the number of stages required for a specified separation. They are strictly what are referred to as "rating methods" and are used to determine the performance of existing, or specified, columns. Given the number of stages, they can be used to determine product compositions. Iterative procedures are necessary to apply rating methods to the design of new columns. Shortcut models can be used to generate initial estimates of the number of stages and feed stage, as described earlier and in Section 4.5.2. If a good initial estimate is provided, the rigorous model should converge faster and can be used to size and optimize the column.

17.8.1 Linear algebra (simultaneous) methods

If the equilibrium relationships and flow rates are known (or assumed), the set of material balance equations for each component is linear in the component compositions. Amundson and Pontinen (1958) developed a method in which these equations are solved simultaneously and the results used to provide improved estimates of the temperature and flow profiles. The set of equations can be expressed in matrix form and solved using standard inversion routines. Convergence can usually be achieved after a few iterations and can be improved by use of Newton's method.

This approach has been further developed by other workers, notably Wang and Henke (1966) and Naphtali and Sandholm (1971). The Naphtali and Sandholm method for solving rigorous columns is available in many commercial simulation programs.

17.8.2 Inside-out algorithms

The inside-out algorithms accelerate convergence by decomposing the solution of the MESH equations into two nested iteration loops. The method was initially proposed by Boston and Sullivan (1974) and has undergone many improvements; see Boston (1980).

The outer iteration loop determines local estimates of K values and stream enthalpies using models that depend on composition and temperature. The local model parameters are the iteration variables for the outside loop. The initial estimates for the outside loop come from the initial estimate of composition and temperature profile supplied by the user.

The inner iteration loop contains the MESH equations, expressed in terms of the local physical property parameters obtained from the outer loop. With simplified physical property models, the inner loop can be converged more quickly. Convergence methods such as bounded Wegstein and Broyden quasi-Newton are typically used, as described in Section 4.7.2.

When the inside loop is converged, the new estimates of composition and temperature are used to update the outer loop parameters. The convergence tolerance of the inside loop is usually tightened at each iteration of the outside loop. The outer loop converges when the changes in local model parameters are within a satisfactory tolerance from one iteration to the next.

All of the commercial process simulation programs offer inside-out algorithms, and some offer several variants that use different convergence methods. Inside-out algorithms are very effective if good initial estimates are provided. Because of their robust and rapid convergence, they are usually the default methods recommended by the simulation program.

Inside-out algorithms can be difficult to converge if no estimate of the temperature profile is provided, so the design engineer should always enter an estimated temperature profile. Shortcut methods can be used to obtain initial estimates of composition and temperature profiles. Another effective strategy is to initialize the model using specifications that are easily met, such as reflux ratio and bottoms flow, and then use the resulting temperature and composition profiles as initial estimates for a simulation with the required purity or recovery specifications.

17.8.3 Relaxation methods

With the exception of this method, all the methods described solve the stage equations for the steady-state design conditions. In an operating column other conditions will exist at start-up, and the column will approach the "design" steady-state conditions after a certain period. The stage material balance equations can be written in a finite difference form, and procedures for the solution of these equations will model the unsteady-state behavior of the column.

Rose et al. (1958) and Hanson and Sommerville (1963) have applied "relaxation methods" to the solution of the unsteady-state equations to obtain the steady-state values. The application of this method to the design of multistage columns is described by Hanson and Sommerville (1963). They give a program listing and worked examples for a distillation column with side streams and for a reboiled absorber.

Relaxation methods are not competitive with the "steady-state" methods in the use of computer time because of slow convergence. However, because they model the actual operation of the column, convergence should be achieved for all practical problems. Relaxation methods are used for dynamic simulation of distillation and for rate-based models such as Aspen Plus RateFrac and BatchFrac. Dynamic models are very useful when attempting to understand the control and operation of distillation columns.

17.9 Other distillation processes

17.9.1 Batch distillation

In batch distillation the mixture to be distilled is charged as a batch to the still and the distillation carried out until a satisfactory top or bottom product is achieved. The still usually consists of a vessel surmounted by a packed or plate column. The heater may be incorporated in the vessel or a separate reboiler used. Batch distillation should be considered under the following circumstances:

1. Where the quantity to be distilled is small
2. Where a range of products has to be produced
3. Where the feed is produced at irregular intervals
4. Where batch integrity is important
5. Where the feed composition varies over a wide range

When the choice between batch and continuous distillation is uncertain, an economic evaluation of both systems should be made.

Batch distillation is an unsteady-state process, the composition in the still (bottoms) varying as the batch is distilled.

Two modes of operation are used:

1. Fixed reflux, where the reflux rate is kept constant. The compositions will vary as the more volatile component is distilled off, and the distillation is stopped when the average composition of the distillate collected, or the bottoms left, meet the specification required.
2. Variable reflux, where the reflux rate is varied throughout the distillation to produce a fixed overhead composition. The reflux ratio will need to be progressively increased as the fraction of the more volatile component in the base of the still decreases.

The basic theory of batch distillation is given in Chhabra and Gurappa (2019) and in several other texts: Hart (1997), Green and Southard (2018), and Couper et al. (2012). In the simple theoretical analysis of batch distillation columns, the liquid hold-up in the column is usually ignored. This hold-up can have a significant effect on the separating efficiency and should be taken into account when designing batch distillation columns. The practical design of batch distillation columns is covered by Hengstebeck (1976), Ellerbe (1997), and Hart (1997).

17.9.2 Vacuum distillation

Components that boil at high temperatures or suffer thermal degradation are sometimes distilled under vacuum to reduce the temperature required for distillation. Vacuum distillation is more expensive than steam distillation, but can be used for compounds that are miscible with water or for processes where the introduction of water might lead to problems such as the formation of azeotropes. The vacuum is usually generated using a vacuum pump or an ejector system on the column overhead product. Selection and design of vacuum pumps and ejectors are described in Chapter 20.

Vacuum columns have high capital and operating costs for the following reasons:

1. Low pressure decreases vapor density, so the column diameter is increased.
2. The vacuum production equipment has high capital and operating costs.
3. The column must be designed to withstand an external pressure. Thicker walls are required for vessels subject to external pressure, as described in Section 14.7.
4. Additional safety precautions and inspection are needed to ensure air cannot enter the equipment if the process fluids are flammable.

Because vacuum columns need low pressure drop per tray, low weir heights are used for plate columns, leading to low stage efficiency and a need for more trays. Packings are therefore often preferred for vacuum service.

17.9.3 Steam distillation

In steam distillation, steam is introduced into the column to lower the partial pressure of the volatile components. Steam distillation is used for the distillation of heat-sensitive products and for compounds with a high boiling point. It is an alternative to vacuum distillation. The products must be immiscible with water. Some steam will normally be allowed to condense to provide the heat required for the distillation. Live steam can be injected directly into the column base, or the steam can be generated by a heater in the still or in an external boiler.

The design procedure for columns employing steam distillation is essentially the same as that for conventional columns, making allowance for the presence of steam in the vapor.

Steam distillation is used extensively in the extraction of essential oils from plant materials.

17.9.4 Reactive distillation

Reactive distillation is the name given to a process where the chemical reaction and product separation are carried out simultaneously in one vessel. Carrying out the reaction, with separation and purification of the product by distillation, gives the following advantages:

1. Chemical equilibrium restrictions can be overcome if a product is removed as it is formed.
2. Energy savings can be obtained if the heat of reaction can be used for the distillation.
3. Capital costs are reduced, as only one vessel is required.

The design of reactive distillation columns is complicated by the complex interactions between the reaction and separation processes. Detailed discussion of reactive distillation is given by Towler and Frey (2002) and Sundmacher and Kiene (2003).

Reactive distillation is used in the production of MTBE (methyl tertiary butyl ether) and methyl acetate.

17.9.5 Petroleum fractionation

Petroleum mixtures such as crude oil and the products of oil refining processes contain from 10^2 to greater than 10^5 components, typically including almost every possible hydrocarbon isomer in the boiling range of the mixture. It is usually neither necessary nor desirable to separate these mixtures into pure components, as the processing goal is to form mixtures with suitable properties, such as volatility and viscosity, for use as fuels. The mixture is distilled into *fractions* or *cuts* that have a suitable boiling range for blending into a fuel or sending for additional processing. The distillation of mineral oils is therefore known as *fractionation*, although this term is sometimes also applied to conventional multicomponent distillation.

The specifications for fractionation columns are usually not set in terms of key components. Instead, the designer specifies cut points for the product streams. The cut points are points on the product stream boiling curve, typically at 5% and 95% of the total material distilled. The sharpness of separation between two fractions is then measured by the overlap between the 95% cut temperature of the lighter fraction and the 5% cut temperature of the heavy fraction.

A good introduction to petroleum fractionation is given by Watkins (1979).

The simulation of petroleum fractionation columns is discussed in Sections 4.4.2 and 4.5.2. Most of the commercial process simulation programs incorporate prebuilt complex column configurations for petroleum fractionation and also have standard sets of pseudocomponents that can be used to fit the feed and product boiling curves.

17.10 Plate efficiency

The designer is concerned with real contacting stages, not the theoretical equilibrium stage assumed for convenience in the mathematical analysis of multistage processes. Equilibrium will rarely be attained in a real stage. The concept of stage efficiency is used to link the performance of practical contacting stages to the theoretical equilibrium stage.

Three principal definitions of efficiency are used:

1. Murphree plate efficiency (Murphree, 1925), defined in terms of the vapor compositions by:

$$E_{mV} = \frac{y_n - y_{n-1}}{y_e - y_{n-1}} \tag{17.31}$$

   where y_e is the composition of the vapor that would be in equilibrium with the liquid leaving the plate. The Murphree plate efficiency is the ratio of the actual separation achieved to that which would be achieved in an equilibrium stage (see Fig. 17.8). In this definition of efficiency, the liquid and the vapor stream are taken to be perfectly mixed; the compositions in Equation 17.31 are the average composition values for the streams.
2. Point efficiency (Murphree point efficiency). If the vapor and liquid compositions are taken at a point on the plate, Equation 17.31 gives the local or point efficiency, *Emv*.
3. Overall column efficiency. This is sometimes confusingly referred to as the overall plate efficiency.

$$E_o = \frac{\text{number of ideal stages}}{\text{number of real stages}} \tag{17.32}$$

An estimate of the overall column efficiency will be needed when the design method used gives an estimate of the number of ideal stages required for the separation.

In some methods, the Murphree plate efficiencies can be incorporated into the procedure for calculating the number of stages and the number of real stages determined directly.

For the idealized situation where the operating and equilibrium lines are straight, the overall column efficiency and the Murphree plate efficiency are related by an equation derived by Lewis (1936):

$$E_0 = \frac{\log\left[1 + E_{mV}\left(\frac{mV}{L} - 1\right)\right]}{\log\left(\frac{mV}{L}\right)} \tag{17.33}$$

where m = slope of the equilibrium line
V = molar flow rate of the vapor
L = molar flow rate of the liquid

Equation 17.33 is not of much practical use in distillation, as the slopes of the operating and equilibrium lines will vary throughout the column. It can be used by dividing the column into sections and calculating the slopes over each section. For most practical purposes, providing the plate efficiency does not vary too much, a simple average of the plate efficiency calculated at the column top, bottom, and feed points will be sufficiently accurate.

17.10.1 Prediction of plate efficiency

Whenever possible, the plate efficiencies used in design should be based on measured values for similar systems obtained on full-sized columns. There is no entirely satisfactory method for predicting plate efficiencies from the system physical properties and plate design parameters; however, the methods given in this section can be used to make a rough estimate where no reliable experimental values are available. They can also be used to extrapolate data obtained from small-scale experimental columns. If the system properties are at all unusual, experimental confirmation of the predicted values should always be obtained. The small, laboratory-scale, glass sieve plate column developed by Oldershaw (1941) has been shown to give reliable values for scale-up. The use of Oldershaw columns is described in papers by Swanson and Gester (1962), Veatch et al. (1960), and Fair et al. (1983).

Some typical values of plate efficiency for a range of systems are given in Table 17.1. More extensive compilations of experimental data are given by Vital et al. (1984) and Kister (1992).

Plate, and overall column, efficiencies will normally be between 30% and 80%, and as a rough guide a figure of 70% can be assumed for preliminary designs. Efficiencies will be lower for vacuum distillations, as low weir heights are used to keep the pressure drop small (see Section 17.10.4).

Multicomponent systems

The prediction methods given in the following sections, and those available in the open literature, are usually restricted to binary systems. It is clear that in a binary system the efficiency obtained for each component must be the same. This is not so for a multicomponent system; the heavier components will usually exhibit lower efficiencies than the lighter components.

The following guide rules, adapted from a paper by Toor and Burchard (1960), can be used to estimate the efficiencies for a multicomponent system from binary data:

1. If the components are similar, the multicomponent efficiencies will be similar to the binary efficiency.
2. If the predicted efficiencies for the binary pairs are high, the multicomponent efficiency will be high.
3. If the resistance to mass transfer is mainly in the liquid phase, the difference between the binary and multicomponent efficiencies will be small.
4. If the resistance is mainly in the vapor phase, as it normally will be, the difference between the binary and multicomponent efficiencies can be substantial.

The prediction of efficiencies for multicomponent systems is also discussed by Chan and Fair (1984b). For mixtures of dissimilar compounds, the efficiency can be quite different from that predicted for each binary pair, and laboratory or pilot-plant studies should be made to confirm any predictions.

17.10.2 O'Connell's correlation

A quick estimate of the overall column efficiency can be obtained from the correlation given by O'Connell (1946), which is shown in Fig. 17.19. The overall column efficiency is correlated with the product of the relative volatility of the light key component (relative to the heavy key) and the molar average viscosity of the feed, estimated at the

TABLE 17.1 Representative efficiencies, sieve plates

System	Column dia., m	Pressure kPa, abs	Efficiency % E_{mV}	Efficiency % E_o
Water–methanol	1.0	—	80	
Water–ethanol	0.2	101	90	
Water–isopropanol	—	—		70
Water–acetone	0.15	90	80	
Water–acetic acid	0.46	101	75	
Water–ammonia	0.3	101	90	
Water–carbon dioxide	0.08	—	80	
Toluene–propanol	0.46	—	65	
Toluene–ethylene dichloride	0.05	101		75
Toluene –methylethylketone	0.15	—		85
Toluene–cyclohexane	2.4	—		70
Toluene –methylcyclohexane	—	27		90
Toluene–octane	0.15	101		40
Heptane–cyclohexane	1.2	165	95	85
	2.4	165		75
Propane–butane	—	—		100
Isobutane–n-butane	—	2070		110
Benzene–toluene	0.13	—	75	
Benzene–methanol	0.18	690	94	
Benzene–propanol	0.46	—	55	
Ethylbenzene–styrene	—	—	75	

E_{mV} = Murphree plate efficiency.
E_o = *Overall column efficiency*.

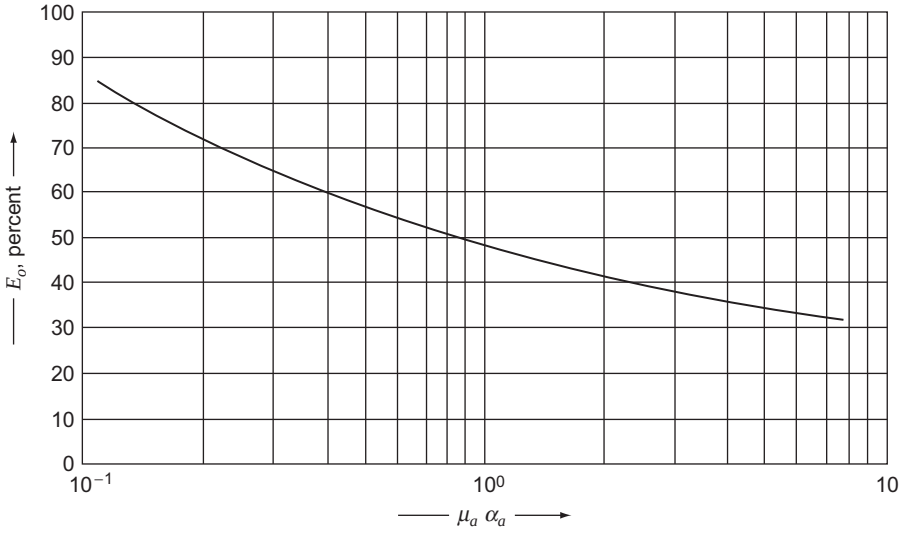


FIG. 17.19 Distillation column efficiencies (bubble-caps). *(From O'Connell, 1946.)*

average column temperature. The correlation was based mainly on data obtained with hydrocarbon systems, but includes some values for chlorinated solvents and water–alcohol mixtures. It has been found to give reliable estimates of the overall column efficiency for hydrocarbon systems and can be used to make an approximate estimate of the efficiency for other systems. The method takes no account of the plate design parameters and includes only two physical property variables.

The O'Connell correlation is the most widely used method for estimating stage efficiency in industrial practice. The calculation is much simpler than the more sophisticated methods that follow, and the results are good enough for most design purposes. The relationship between the O'Connell correlation and the more theoretical methods is discussed by Duss and Taylor (2018). They also discuss situations where the O'Connell correlation is not applicable.

Eduljee (1958) has expressed the O'Connell correlation in the form of an equation:

$$E_o = 51 - 32.5 \log(\mu_a \alpha_a) \tag{17.34}$$

where μ_a = the molar average liquid viscosity, mNs/m^2
α_a = average relative volatility of the light key

Absorbers

O'Connell gave a similar correlation for the plate efficiency of absorbers (Fig. 17.20). Appreciably lower plate efficiencies are obtained in absorption than in distillation.

In O'Connell's paper, the plate efficiency is correlated with a function involving Henry's constant, the total pressure, and the solvent viscosity at the operating temperature.

To convert the original data to SI units, it is convenient to express this function in the following form:

$$x = 0.062\left[\frac{\rho_s P}{\mu_s \mathrm{H} M_s}\right] = 0.062\left[\frac{\rho_s}{\mu_s K M_s}\right] \tag{17.35}$$

where H = the Henry's law constant, Nm^{-2}/mol fraction
P = total pressure, N/m^2
μ_s = solvent viscosity, mNs/m^2
M_s = molecular weight of the solvent
ρ_s = solvent density, kg/m^3
K = equilibrium constant for the solute

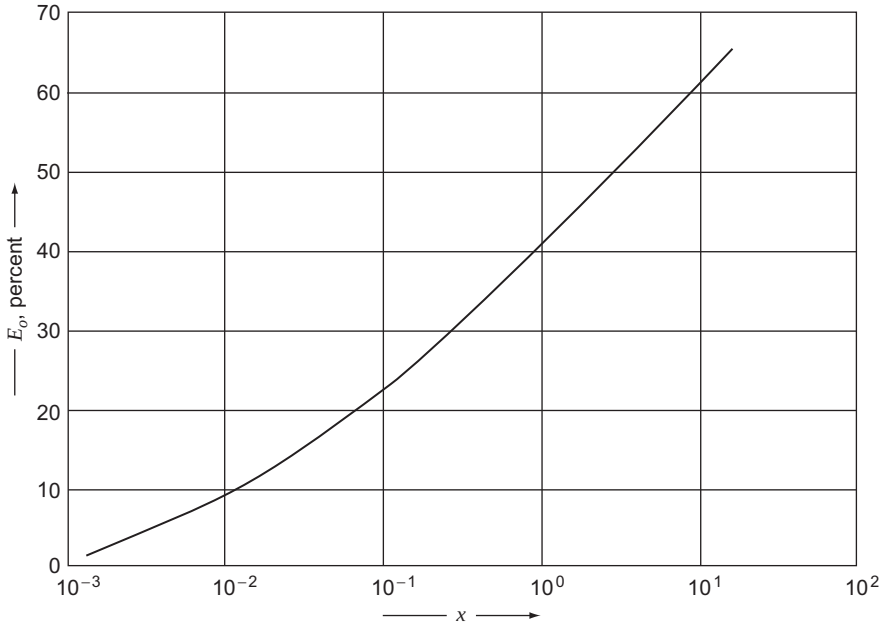


FIG. 17.20 Absorber column efficiencies (bubble-caps). *(From O'Connell, 1946.)*

Example 17.5

Using O'Connell's correlation, estimate the overall column efficiency and the number of real stages required for the separation given in Example 17.3 when the reflux ratio is 2.0.

Solution

From Example 17.3, feed composition, mol fractions:

Propane 0.05, i-butane 0.15, n-butane 0.25, i-pentane 0.20, n-pentane 0.35
Column-top temperature 65 °C, bottom temperature 120 °C
Average relative volatility light key = 2.0
Take the viscosity at the average column temperature, 93 °C:
viscosities, propane = 0.03 mNs/m^2
butane = 0.12 mNs/m^2
pentane = 0.14 mNs/m^2

For feed composition, molar average viscosity $= 0.03 \times 0.05 + 0.12(0.15 + 0.25)$:

$$+0.14(0.20+0.35)$$
$$= 0.13 \text{ mNs/m}^2$$
$$\alpha_a \mu_a = 2.0 \times 0.13 = 0.26$$

From Fig. 17.19, $E_o = \underline{\underline{70}}\%$

From Example 17.3, when the reflux ratio is 2.0, number of ideal stages = 16, one ideal stage will be the reboiler, so number of actual stages (rounding up):

$$= \frac{(16 - 1)}{0.7} = \underline{\underline{22}}$$

17.10.3 Van Winkle's correlation

Van Winkle et al. (1972) have published an empirical correlation for the plate efficiency that can be used to predict plate efficiencies for binary systems. Their correlation uses dimensionless groups that include those system variables and plate parameters that are known to affect plate efficiency. They give two equations, the simplest, and that which they consider the most accurate, is given here. The data used to derive the correlation covered both bubble-cap and sieve plates.

$$E_{mV} = 0.07 \text{Dg}^{0.14} \text{Sc}^{0.25} \text{Re}^{0.08} \tag{17.36}$$

where Dg = surface tension number = $(\sigma_L / \mu_L u_v)$
u_v = superficial vapor velocity
σ_L = liquid surface tension
μ_L = liquid viscosity
Sc = liquid Schmidt number = $(\mu_L / \rho_L D_{LK})$
ρ_L = liquid density
D_{LK} = liquid diffusivity, light key component
Re = Reynolds number = $(h_w u_v \rho_v / \mu_L (\text{FA}))$
h_w = weir height
ρ_v = vapor density

$$(\text{FA}) = \text{fractional area} = \frac{(\text{area of holes or risers})}{(\text{total column cross} - \text{sectional area})}$$

The use of this method is illustrated in Example 17.8.

17.10.4 AIChE method

This method of predicting plate efficiency, published in 1958, was the result of a 5-year study of bubble-cap plate efficiency directed by the Research Committee of the American Institute of Chemical Engineers. The AIChE method is the most detailed method for predicting plate efficiencies that is available in the open literature. It takes into account all the major factors that are known to affect plate efficiency, including:

- The mass transfer characteristics of the liquid and vapor phases
- The design parameters of the plate
- The vapor and liquid flow rates
- The degree of mixing on the plate

The method is well established, and in the absence of experimental values, or proprietary prediction methods, should be used when more than a rough estimate of efficiency is needed.

The approach taken is semi-empirical. Point efficiencies are estimated making use of the "two-film theory" and the Murphree efficiency estimated allowing for the degree of mixing likely to be obtained on real plates.

The procedure and equations are given in this section without discussion of the theoretical basis of the method. The reader should refer to the AIChE manual (1958) or to Smith (1963), who gives a comprehensive account of the method and extends its use to sieve plates. Chan and Fair (1984a) published an alternative method for point efficiencies on sieve plates, which they demonstrate gives closer predictions than the AIChE method. The Chan and Fair method follows the same overall methodology as the AIChE method but uses an improved correlation for vapor phase mass transfer, given later.

AIChE method

The mass transfer resistances in the vapor and liquid phases are expressed in terms of the number of transfer units, $\mathbf{N}_G$ and $\mathbf{N}_L$. The point efficiency is related to the number of transfer units by the equation:

$$\frac{1}{\ln(1 - E_{mv})} = -\left[\frac{1}{\mathbf{N}_G} + \frac{mV}{L} \times \frac{1}{\mathbf{N}_L}\right] \tag{17.37}$$

where m is the slope of the equilibrium line and V and L the vapor and liquid molar flow rates.

Equation 17.37 is plotted in Fig. 17.21.

The number of gas-phase transfer units in the AIChE method is given by:

$$\mathbf{N}_G = \frac{(0.776 + 4.57 \times 10^{-3} h_w - 0.24F_v + 105L_p)}{\left(\frac{\mu_v}{\rho_v D_v}\right)^{0.5}} \tag{17.38}$$

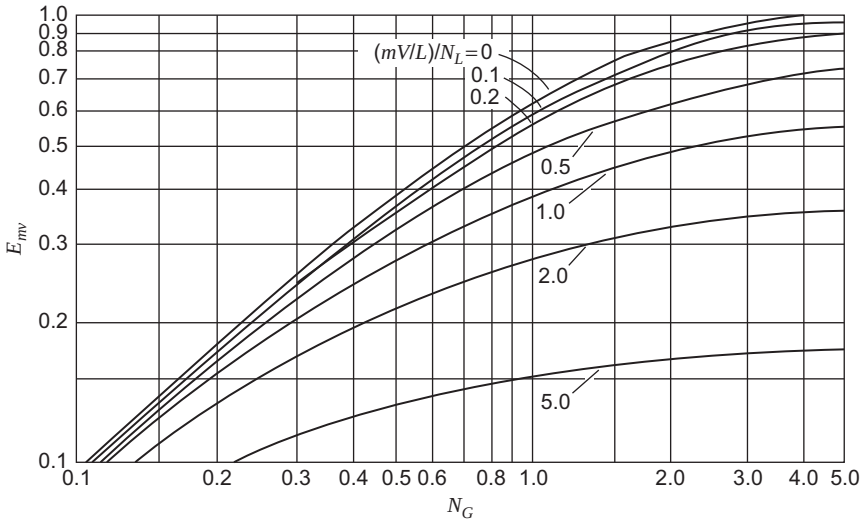


FIG. 17.21 Relationship between point efficiency and number of liquid and vapor transfer units (Equation 17.37).

where h_w = weir height, mm.
F_v = the column vapor "F" factor = $u_a\ \rho_v^{0.5}$.
u_a = vapor velocity based on the active tray area (bubbling area), see Section 17.13.2, m/s.
L_p = the volumetric liquid flow rate across the plate, divided by the average width of the plate,m^3/sm. The average width can be calculated by dividing the active area by the length of the liquid path Z_L.
μ_v = vapor viscosity, Ns/m^2.
ρ_v = vapor density; kg/m^3.
D_v = vapor diffusivity, m^2/s.

In the alternative method proposed by Chan and Fair (1984a), the number of gas-phase mass transfer units is given by:

$$\mathbf{N}_G = \frac{D_v^{0.5}(1030f - 867f^2)\ \overline{t_v}}{h_L{}^{0.5}} \tag{17.39}$$

where h_L = liquid hold-up on tray, cm
$\overline{t_v}$ = average vapor residence time, s
$f = u_a / u_{af}$ = fractional approach to the vapor velocity based on active area at flooding, u_{af}

The remainder of the Chan and Fair method is the same as the AIChE method.
In both methods, the number of liquid-phase transfer units is given by:

$$\mathrm{N}_L = \left(4.13 \times 10^8 D_L\right)^{0.5} (0.21\mathrm{F}_v + 0.15)t_L \tag{17.40}$$

where D_L = liquid-phase diffusivity, m^2/s
t_L = liquid contact time, s
given by:

$$t_L = \frac{Z_c Z_L}{L_p} \tag{17.41}$$

where Z_L = length of the liquid path from inlet downcomer to outlet weir, m
Z_c = liquid hold-up on the plate, m^3 per m^2 active area
given by:
for bubble-cap plates:

$$Z_c = 0.042 + 0.19 \times 10^{-3} h_w - 0.014F_v + 2.5L_p \tag{17.42}$$

for sieve plates:

$$Z_c = 0.006 + 0.73 \times 10^{-3} h_w - 0.24 \times 10^{-3} F_v h_w + 1.22L_p \tag{17.43}$$

The Murphree efficiency E_{mV} is only equal to the point efficiency E_{mv} if the liquid on the plate is perfectly mixed. On a real plate this will not be so, and to estimate the plate efficiency from the point efficiency, some means of estimating the degree of mixing is needed. The dimensionless Peclet number characterizes the degree of mixing in a system. For a plate, the Peclet number is given by:

$$\mathrm{Pe} = \frac{Z_L^2}{D_e\ t_L} \tag{17.44}$$

where D_e is the "eddy diffusivity", m^2/s.
A Peclet number of zero indicates perfect mixing, and a value of ∞ indicates plug flow.
For bubble-cap and sieve plates, the eddy diffusivity can be estimated from the equation:

$$D_e = \left(0.0038 + 0.017u_a + 3.86L_p + 0.18 \times 10^{-3} h_w\right)^2 \tag{17.45}$$

The relation between the plate efficiency and point efficiency with the Peclet number as a parameter is shown in Fig. 17.22. The application of the AIChE method is illustrated in Example 17.7.

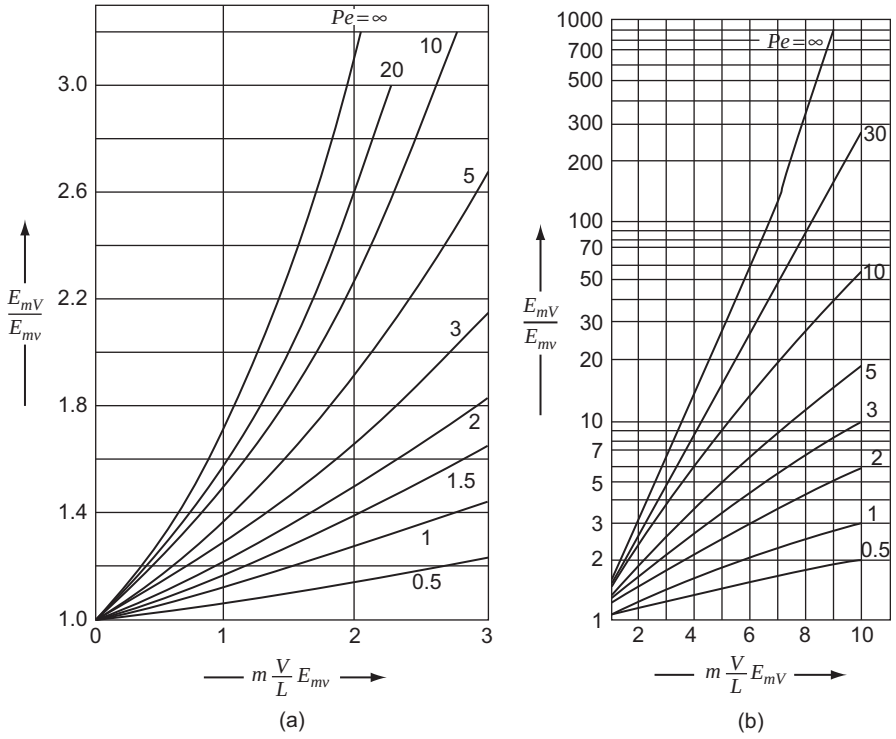


FIG. 17.22 Relationship between plate and point efficiency.

Estimation of physical properties

To use the AIChE method or Van Winkle's correlation, estimates of the physical properties are required. It is unlikely that experimental values will be found in the literature for all systems that are of practical interest. The prediction methods given in Chapter 4, and in the references given in that chapter, can be used to estimate values.

The AIChE design manual recommends the Wilke and Chang (1955) equation for liquid diffusivities (see Section 15.3.4) and the Wilke and Lee (1955) modification to the Hirschfelder, Bird, and Spotz equation for gas diffusivities.

Plate design parameters

The significance of the weir height in the AIChE equations should be noted. The weir height was the plate parameter found to have the strongest effect on plate efficiency. Increasing weir height will increase the plate efficiency, but at the expense of an increase in pressure drop and entrainment. Weir heights will normally be in the range 40 to 100 mm for columns operating at and above atmospheric pressure, but will be as low as 6 mm for vacuum columns. This largely accounts for the lower plate efficiencies obtained in vacuum columns.

The length of the liquid path Z_L is taken into account when assessing the plate mixing performance. The mixing correlation given in the AIChE method was not tested on large-diameter columns, and Smith (1963) states that the correlation should not be used for large-diameter plates; however, on a large plate the liquid path will normally be subdivided, and the value of Z_L will be similar to that in a small column. The assumption that the vapor space is well-mixed across the tray may also not be valid for large column diameters.

The vapor "F" factor F_v is a function of the active tray area. Increasing F_v decreases the number of gas-phase transfer units. The liquid flow term L_p is also a function of the active tray area and the liquid path length. It will only have a significant effect on the number of transfer units if the path length is long. In practice, the range of values for F_v, the active area, and the path length will be limited by other plate design considerations.

Multicomponent systems

The AIChE method was developed from measurements on binary systems. The AIChE manual should be consulted for advice on its application to multicomponent systems. See also the comments in Section 17.10.1.

17.10.5 Entrainment

The AIChE method and that of Van Winkle predict the "dry" Murphree plate efficiency. In operation some liquid droplets will be entrained and carried up the column by the vapor flow, and this will reduce the actual, operating, efficiency.

The dry-plate efficiency can be corrected for the effects of entrainment using the equation proposed by Colburn (1936):

$$E_a = \frac{E_{mV}}{1 + E_{mV}\left[\dfrac{\psi}{1-\psi}\right]} \tag{17.46}$$

where E_a = actual plate efficiency, allowing for entrainment

$$\Psi = \text{the fractional entrainment} = \frac{\text{entrained liquid}}{\text{gross liquid flow}}$$

A method for predicting the entrainment from sieve plates is given in Section 17.13.5, Fig. 17.36; a similar method for bubble-cap plates is given by Bolles (1963).

17.11 Approximate column sizing

An approximate estimate of the overall column size can be made once the number of real stages required for the separation is known. This is often needed to make a rough estimate of the capital cost for project evaluation.

Plate spacing

The overall height of the column will depend on the plate spacing. Plate spacings from 0.15 m (6 in) to 1 m (36 in) are normally used. The spacing chosen will depend on the column diameter and operating conditions. Close spacing is used with small-diameter columns, and where head room is restricted; as it will be when a column is installed in a building. For columns above 1 m in diameter, plate spacings of 0.3 to 0.6 m will normally be used, and 0.5 m (18 in) can be taken as an initial estimate. This would be revised, as necessary, when the detailed plate design is made.

A larger spacing will be needed between certain plates to accommodate feed and side-stream arrangements and for manways.

Column diameter

The principal factor that determines the column diameter is the vapor flow rate. The vapor velocity must be below that which would cause excessive liquid entrainment or a high pressure drop. The equation given here, which is based on the well-known Souders and Brown equation, Lowenstein (1961), can be used to estimate the maximum allowable superficial vapor velocity, and hence the column area and diameter:

$$\hat{u}_v = \left(-0.171 l_t^2 + 0.27 l_t - 0.047\right)\left[\frac{\rho_L - \rho_v}{\rho_v}\right]^{1/2} \tag{17.47}$$

where $\hat{u}_v$ = maximum allowable vapor velocity, based on the gross (total) column cross-sectional area, m/s
l_t = plate spacing, m (range 0.5 to 1.5)

The column diameter, D_c, can then be calculated:

$$D_c = \sqrt{\frac{4\hat{V}_w}{\pi \rho_v \hat{u}_v}} \tag{17.48}$$

where $\hat{V}_w$ is the maximum vapor rate, kg/s.

This approximate estimate of the diameter would be revised when the detailed plate design is undertaken.

The column diameter estimated should then be rounded up to the nearest standard head size so that preformed heads can be used as vessel closures; see Section 14.5.2. The column sizing programs in most commercial process simulation programs use North American standard head sizes, which are available in 6-in (152.4-mm) increments.

17.12 Plate contactors

Cross-flow plates are the most common type of plate contactor used in distillation and absorption columns. In a cross-flow plate the liquid flows across the plate and the vapor up through the plate. A typical layout is shown in Fig. 17.23. The flowing liquid is transferred from plate to plate through vertical channels called "downcomers." A pool of liquid is retained on the plate by an outlet weir.

Other types of plate are used that have no downcomers (non-cross-flow plates), with the liquid showering down the column through large openings in the plates (sometimes called shower plates). These and other proprietary non-cross-flow plates are used for special purposes, particularly when a low-pressure drop is required.

Four principal types of cross-flow tray are used, classified according to the method used to contact the vapor and liquid.

1. Sieve plate (perforated plate) (Fig. 17.24)

This is the simplest type of cross-flow plate. The vapor passes up through perforations in the plate, and the liquid is retained on the plate by the vapor flow. There is no positive vapor–liquid seal, and at low flow rates liquid will "weep" through the holes, reducing the plate efficiency. The perforations are usually small holes, but larger holes and slots can be used.

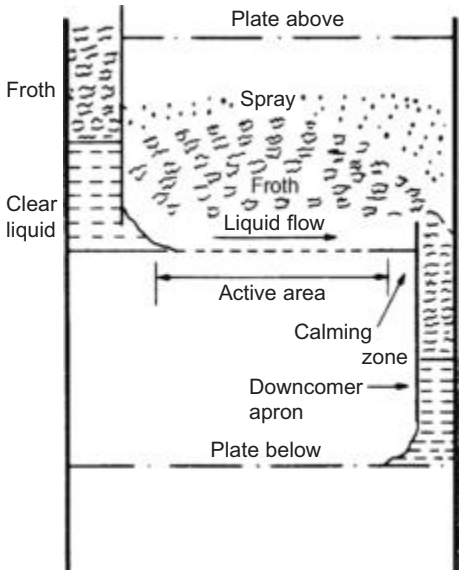


FIG. 17.23 Typical cross-flow plate (sieve).

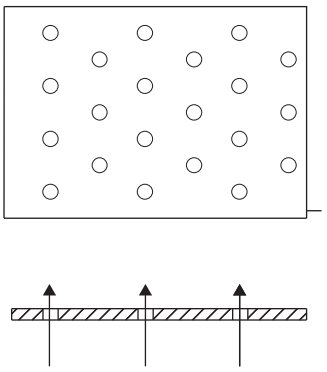


FIG. 17.24 Sieve plate.

2. *Bubble-cap plates (Fig. 17.25)*

Bubble-cap plates are plates in which the vapor passes up through short pipes, called risers, covered by a cap with a serrated edge, or slots. The bubble-cap plate is the traditional, oldest type of cross-flow plate, and many different designs have been developed. Standard cap designs would now be specified for most applications.

The most significant feature of the bubble-cap plate is that the use of risers ensures that a level of liquid is maintained on the tray at all vapor flow rates. Bubble-caps therefore have good turndown performance at low flow rates. They are more expensive than sieve plates and more prone to corrosion, fouling, and plugging, and so are usually only found on older columns.

3. *Valve plates (floating-cap plates) (Fig. 17.26)*

Valve plates are proprietary designs. They are essentially sieve plates with large-diameter holes covered by movable flaps, which lift as the vapor flow increases.

As the area for vapor flow varies with the flow rate, valve plates can operate efficiently at lower flow rates than sieve plates: the valves closing at low vapor rates. The cost of valve plates is intermediate between sieve plates and bubble-cap plates.

Some very elaborate valve designs have been developed, but the simple type shown in Fig. 17.26 is satisfactory for most applications.

4. *Valve plates (fixed valve plates) (Fig. 17.27)*

A fixed valve plate is similar to a sieve plate, except the holes are only partially punched out, so that the hole remains partially covered, as shown in Fig. 17.27. Fixed valve trays are almost as inexpensive as sieve trays and have improved turndown performance. The relatively small cost difference between fixed valve trays and sieve trays can usually be justified by the improved turndown performance, and fixed valve trays are the most common type specified in nonfouling applications.

Many different proprietary designs of fixed and floating valves have been developed. Performance details can be obtained from the tray vendors.

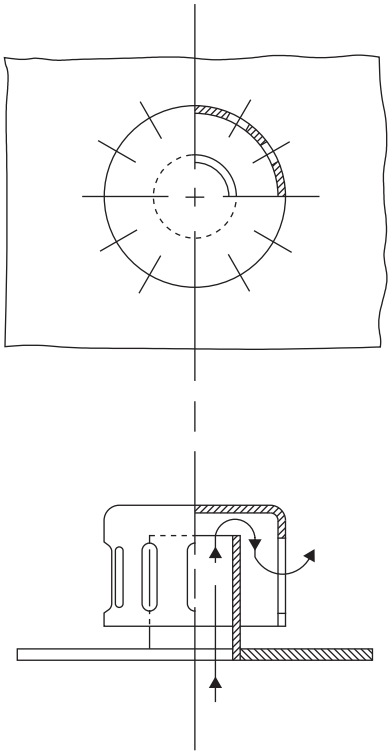


FIG. 17.25 Bubble-cap.

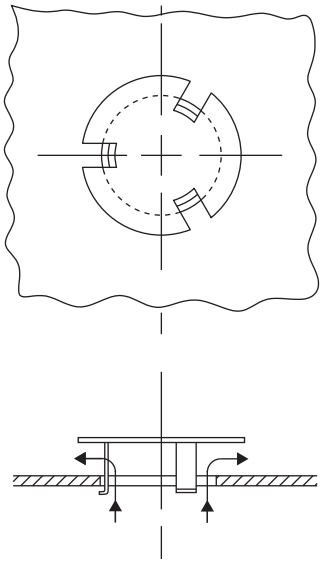


FIG. 17.26 Simple valve.

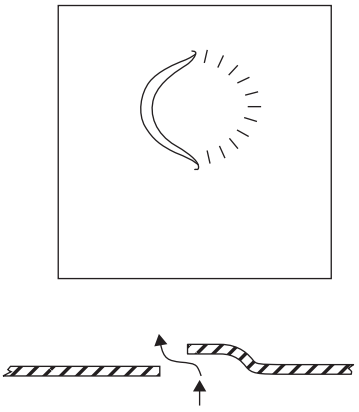


FIG. 17.27 Fixed valve.

Liquid flow pattern

Cross-flow trays are also classified according to the number of liquid passes on the plate. The design shown in Fig. 17.28(a) is a single-pass plate. For low liquid flow rates reverse-flow plates are used (see Fig. 17.28b). In this type the plate is divided by a low central partition and inlet and outlet downcomers are on the same side of the plate. Multiple-pass plates, in which the liquid stream is subdivided by using several downcomers, are used for high liquid flow rates and large-diameter columns. A double-pass plate is shown in Fig. 17.28(c).

Selection of the liquid flow pattern is discussed in Section 17.13.4. An approximate criterion for selecting the liquid flow pattern is the liquid volumetric flow rate per unit weir length, which should ideally be in the range 5 to 8 liters/s per m (2 to 3 gpm/in). Weir length is discussed in more detail in Section 17.13.8.

17.12.1 Selection of plate type

The principal factors to consider when comparing the performance of bubble-cap, sieve, and valve plates are cost, capacity, operating range, efficiency, and pressure drop.

Cost. Bubble-cap plates are appreciably more expensive than sieve or valve plates. The relative cost will depend on the material of construction used; for mild steel, the ratios bubble-cap:valve:fixed valve:sieve are approximately 3.0:1.2:1.1:1.0.

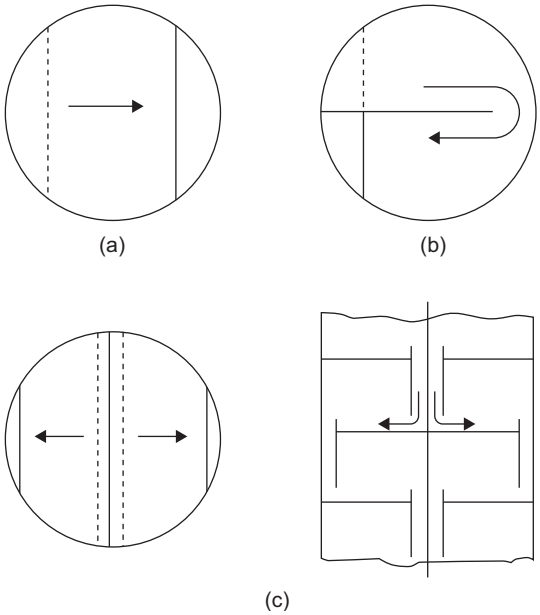


FIG. 17.28 Liquid flow patterns on cross-flow trays. (a) Single pass. (b) Reverse flow. (c) Double pass.

Capacity. There is little difference in the capacity rating of the three types (the diameter of the column required for a given flow rate); the ranking from best to worst is sieve, valve, and bubble-cap.

Operating range. This is the most significant factor. By operating range is meant the range of vapor and liquid rates over which the plate will operate satisfactorily (the stable operating range). Some flexibility will always be required in an operating plant to allow for changes in production rate and to cover start-up and shut-down conditions. The ratio of the highest to the lowest flow rates is often referred to as the "turn-down" ratio. Bubble-cap plates have a positive liquid seal and can therefore operate efficiently at very low vapor rates.

Sieve plates and fixed valve plates rely on the flow of vapor through the holes to hold the liquid on the plate and cannot operate at very low vapor rates. With good design, sieve plates can give a satisfactory operating range; typically, from 50% to 120% of design capacity. Fixed valve plates have somewhat better turndown performance. Valve plates are intended to give greater flexibility than sieve plates at a lower cost than bubble-caps.

Efficiency. The Murphree efficiency of the three types of plate will be virtually the same when operating over their design flow range, and no real distinction can be made between them; see Zuiderweg et al. (1960).

Pressure drop. The pressure drop over the plates can be an important design consideration, particularly for vacuum columns. The plate pressure drop will depend on the detailed design of the plate, but, in general, sieve plates give the lowest pressure drop, followed by valves, with bubble-caps giving the highest.

Summary. Sieve plates are the cheapest and least prone to fouling and are satisfactory for most applications. Fixed valve plates are almost as cheap as sieve plates and have improved turndown behavior. The improved performance usually justifies the increased cost, and this type is most commonly selected for nonfouling applications. Moving valve plates should be considered if the specified turndown ratio cannot be met with sieve plates or fixed valve plates. Bubble-caps should only be used where very low vapor (gas) rates have to be handled and a positive liquid seal is essential at all flow rates.

17.12.2 Plate construction

The mechanical design features of sieve plates are described in this section. The same general construction is also used for bubble-cap and valve plates. Details of the various types of bubble-cap used and the preferred dimensions of standard cap designs can be found in the books by Smith (1963) and Coker (2010). The manufacturers' design manuals should be consulted for details of valve plate design.

Two different types of plate construction are used. Large-diameter plates are normally constructed in sections, supported on beams. Small plates are installed in the column as a stack of preassembled plates.

Sectional construction

A typical plate is shown in Fig. 17.29. The plate sections are supported on a ring welded around the vessel wall and on beams. The beams and ring are about 50 mm wide, with the beams set at around 0.6-m spacing. The beams are usually angle or channel sections, constructed from folded sheet. Special fasteners are used so the sections can be assembled from one side only. One section is designed to be removable to act as a manway. This reduces the number of manways needed on the vessel wall, which reduces the vessel cost.

Stacked plates (cartridge plates)

The stacked type of construction is used where the column diameter is too small for a worker to enter to assemble the plates, say less than 1.2 m (4 ft). Each plate is fabricated complete with the downcomer and joined to the plate above and below using screwed rods (spacers) (Fig. 17.30). The plates are installed in the column shell as an assembly (stack) of 10 or so plates. Tall columns have to be divided into flanged sections so that plate assemblies can be easily installed and removed. The weir and downcomer supports are usually formed by turning up the edge of the plate.

The plates are not fixed to the vessel wall, as they are with sectional plates, so there is no positive liquid seal at the edge of the plate, and a small amount of leakage will occur. In some designs the plate edges are turned up around the circumference to make better contact at the wall. This can make it difficult to remove the plates for cleaning and maintenance without damage.

Downcomers

The segmental, or chord downcomer, shown in Fig. 17.31(a), is the simplest and cheapest form of construction and is satisfactory for most purposes. The downcomer channel is formed by a flat plate, called an apron, which extends down from the outlet weir. The apron is usually vertical, but may be sloped (Fig. 17.31b) to increase the plate area available for perforation. This design is commonly in high-capacity trays. If a more positive seal is required at the downcomer at the outlet, an inlet weir can be fitted (Fig. 17.31c) or a recessed seal pan used (Fig. 17.31d). Circular downcomers (pipes) are sometimes used for small liquid flow rates. Curved downcomers are often used in high-capacity trays for large columns. Truncated downcomers (Fig. 17.31e) can be used to increase the plate area available for perforation and are also commonly used for high-capacity trays.

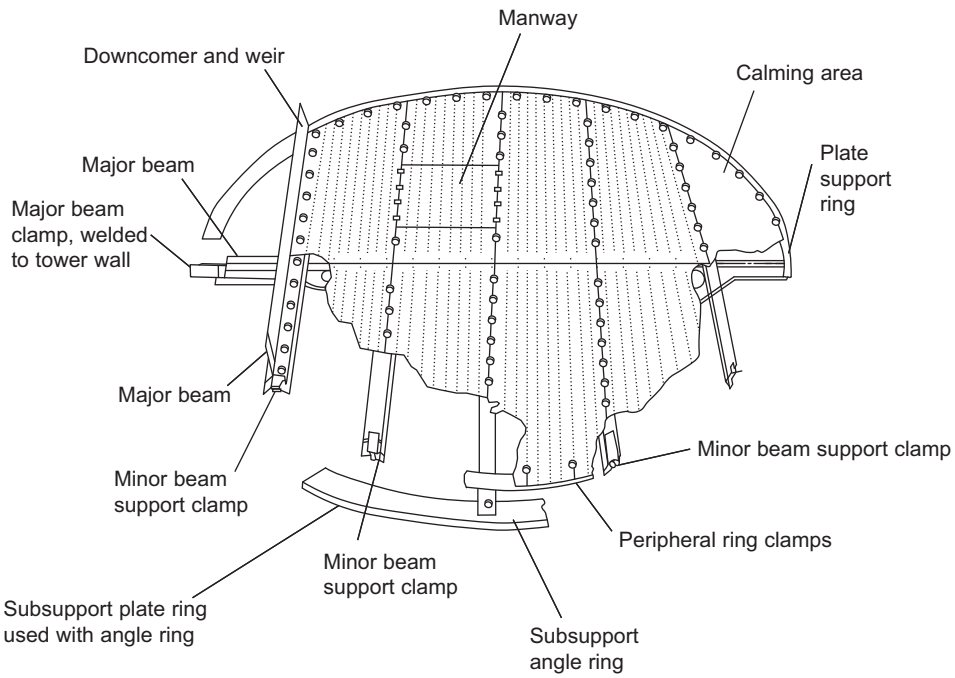


FIG. 17.29 Typical sectional plate construction.

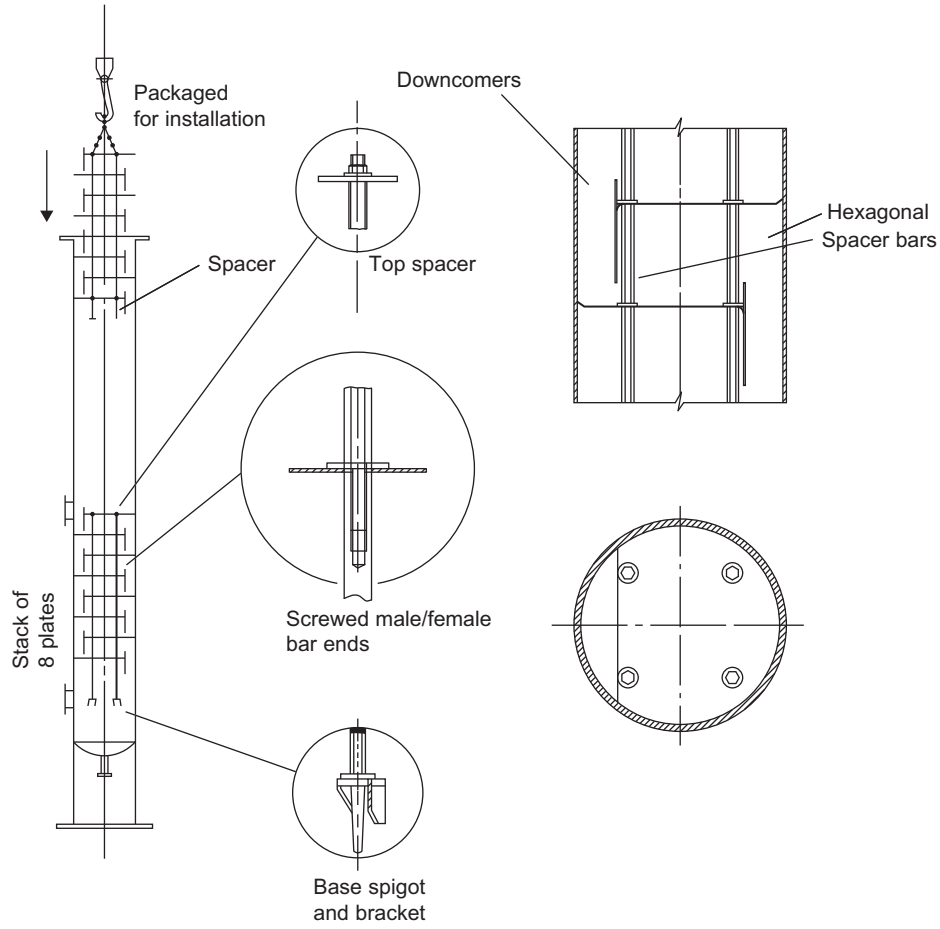


FIG. 17.30 Typical stacked-plate construction.

Side stream and feed points

Where a side stream is withdrawn from the column, the plate design must be modified to provide a liquid seal at the take-off pipe. A typical design is shown in Fig. 17.32(a). Side-draw pipes and run-down lines must be sized for self-venting flow, and provision must be made for vapor to vent from the line in case vapor is entrained from the column or formed by flashing in the line. Sewell (1975) gives a correlation for the minimum pipe diameter that will allow self-venting flow.

When the feed stream is liquid, it will be normally introduced into the downcomer leading to the feed plate and the plate spacing increased at this point (see Fig. 17.32b). This design should not be used if the feed is at the bubble point or is two-phase, as the feed may flash on entering the column, in which case downcomer flooding could occur.

Structural design

The plate structure must be designed to support the hydraulic loads on the plate during operation and the loads imposed during construction and maintenance. Typical design values used for these loads are:

Hydraulic load: 600 N/m^2 live load on the plate, plus 3000 N/m^2 over the downcomer seal area.
Erection and maintenance: 1500 N concentrated load on any structural member.

It is important to set close tolerances on the weir height, downcomer clearance, and plate flatness, to ensure an even flow of liquid across the plate. The tolerances specified will depend on the dimensions of the plate but will typically be about 3 mm.

The plate deflection under load is also important and will normally be specified as not greater than 3 mm under the operating conditions for plates greater than 2.5 m and proportionally less for smaller diameters.

The mechanical specification of bubble-cap, sieve, and valve plates is covered in a series of articles by Glitsch (1960), McClain (1960), Thrift (1960a,b), and Patton and Pritchard (1960).

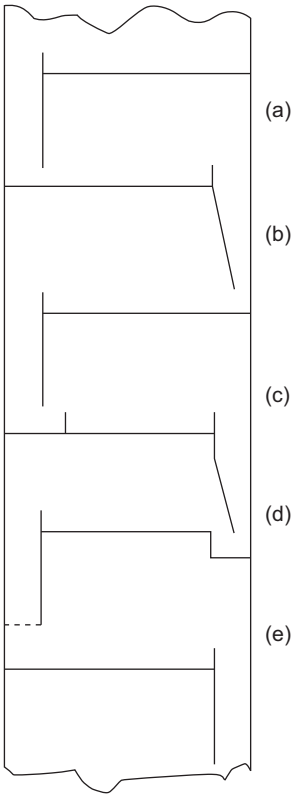


FIG. 17.31 Segment (chord) downcomer designs. (a) Vertical apron. (b) Inclined apron. (c) Inlet weir. (d) Recessed well. (e) Truncated downcomer.

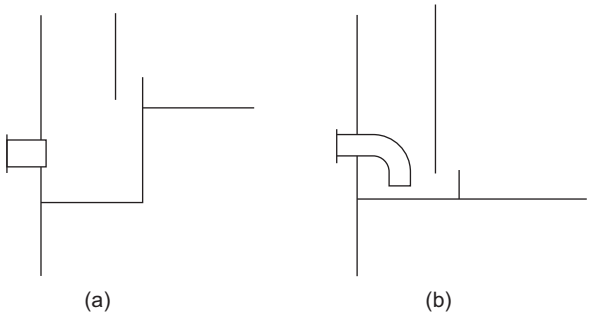


FIG. 17.32 Feed and take-off nozzles.

17.13 Plate hydraulic design

The basic requirements of a plate contacting stage are that it should:

Provide good vapor–liquid contact.
Provide sufficient liquid hold-up for good mass transfer (high efficiency).
Have sufficient area and spacing to keep the entrainment and pressure drop within acceptable limits.
Have sufficient downcomer area for the liquid to flow freely from plate to plate.

Plate design, like most engineering design, is a combination of theory and practice. The design methods use semi-empirical correlations derived from fundamental research work combined with practical experience obtained from the operation of commercial columns. Proven layouts are used, and the plate dimensions are kept within the range of values known to give satisfactory performance.

A short procedure for the hydraulic design of sieve plates is given in this section. Design methods for bubble-cap plates are given by Bolles (1963) and Coker (2010). Valve plates are proprietary designs and will be designed in consultation with the vendors. Design manuals are available from some vendors.

A detailed discussion of the extensive literature on plate design and performance will not be given. Chase (1967) and Zuiderweg (1982) give critical reviews of the literature on sieve plates.

Several design methods have been published for sieve plates: Kister (1992), Barnicki and Davies (1989), Koch and Kuzniar (1966), Fair (1963), and Huang and Hodson (1958); see also the book by Lockett (1986).

Operating range

Satisfactory operation will only be achieved over a limited range of vapor and liquid flow rates. A typical performance diagram for a sieve plate is shown in Fig. 17.33.

The upper limit to vapor flow is set by the condition of flooding. At flooding there is a sharp drop in plate efficiency and an increase in pressure drop. Flooding is caused by either the excessive carryover of liquid to the next plate by entrainment (entrainment or jet flooding) or by liquid backing up in the downcomers.

The lower limit of the vapor flow is set by the condition of weeping. Weeping occurs when the vapor flow is insufficient to maintain a level of liquid on the plate. "Coning" occurs at low liquid rates and is the term given to the condition where the vapor pushes the liquid back from the holes and jets upward, with poor liquid contact.

In the following sections, gas can be taken as synonymous with vapor when applying the method to the design of plates for absorption columns.

17.13.1 Plate design procedure

A trial-and-error approach is necessary in plate design: starting with a rough plate layout, checking key performance factors, and revising the design as necessary until a satisfactory design is achieved. A typical design procedure is set out here and discussed in the following sections. The normal range of each design variable is given in the discussion, together with recommended values that can be used to start the design.

Most of the commercial process simulation programs offer tray design modules. These programs can be used for preliminary tray layout for costing purposes, but the default dimensions selected or calculated by these programs often do not give the best performance over the intended range of operation. An experienced designer will run several cases to confirm the tray performance is satisfactory over the whole range of operation. Hand calculations using the methods given in this section can also be used to guide the process simulation programs to a better design.

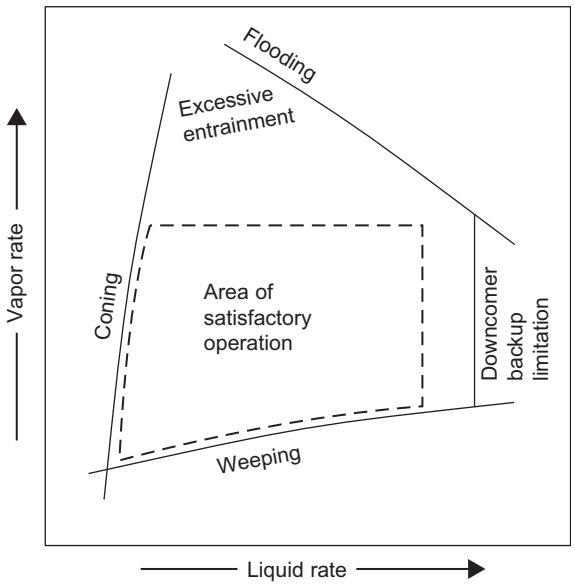


FIG. 17.33 Sieve plate performance diagram.

Procedure

1. Calculate the maximum and minimum vapor and liquid flow rates for the turn-down ratio required.
2. Collect, or estimate, the system physical properties.
3. Select a trial plate spacing (Section 17.11).
4. Estimate the column diameter, based on flooding considerations (Section 17.13.3).
5. Decide the liquid flow arrangement (Section 17.13.4).
6. Make a trial plate layout: downcomer area, active area, hole area, hole size, weir height (Sections 17.13.8 to 17.13.10).
7. Check the weeping rate (Section 17.13.6); if unsatisfactory, return to step 6.
8. Check the plate pressure drop (Section 17.13.14); if too high, return to step 6.
9. Check downcomer backup; if too high, return to step 3 or 6 (Section 17.13.15).
10. Decide plate layout details: calming zones, unperforated areas. Check hole pitch; if unsatisfactory, return to step 6 (Section 17.13.11).
11. Recalculate the percentage flooding based on chosen column diameter.
12. Check entrainment; if too high, return to step 4 (Section 17.13.5).
13. Optimize design: repeat steps 3 to 12 to find smallest diameter and plate spacing acceptable (lowest cost).
14. Finalize design: draw up the plate specification and sketch the layout.

This procedure is illustrated in Example 17.6.

17.13.2 Plate areas

The following area terms are used in the plate design procedure:

A_c = total column cross-sectional area
A_d = cross-sectional area of downcomer
A_n = net area available for vapor–liquid disengagement, normally equal to $A_c - A_d$ for a single-pass plate
A_a = active, or bubbling, area, equal to $A_c - 2A_d$ for single-pass plates
A_h = hole area, the total area of all the active holes
A_p = perforated area (including blanked areas)
A_{ap} = the clearance area under the downcomer apron

17.13.3 Diameter

The flooding condition fixes the upper limit of vapor velocity. A high vapor velocity is needed for high plate efficiencies, and the velocity will normally be between 70% and 90% of that which would cause flooding. For design, a value of 80% to 85% of the flooding velocity should be used.

The flooding velocity can be estimated from the correlation given by Fair (1961):

$$u_f = K_1 \sqrt{\frac{\rho_L - \rho_v}{\rho_v}} \tag{17.49}$$

where u_f = flooding vapor velocity, m/s, based on the net column cross-sectional area A_n (see Section 17.13.2)
K_1 = a constant obtained from Fig. 17.34

The liquid–vapor flow factor F_{LV} in Fig. 17.34 is given by:

$$F_{LV} = \frac{L_w}{V_w} \sqrt{\frac{\rho_v}{\rho_L}} \tag{17.50}$$

where L_w = liquid mass flow rate, kg/s
V_w = vapor mass flow rate, kg/s

The following restrictions apply to the use of Fig. 17.34:

1. Hole size less than 6.5 mm. Entrainment may be greater with larger hole sizes.
2. Weir height less than 15% of the plate spacing.
3. Nonfoaming systems.

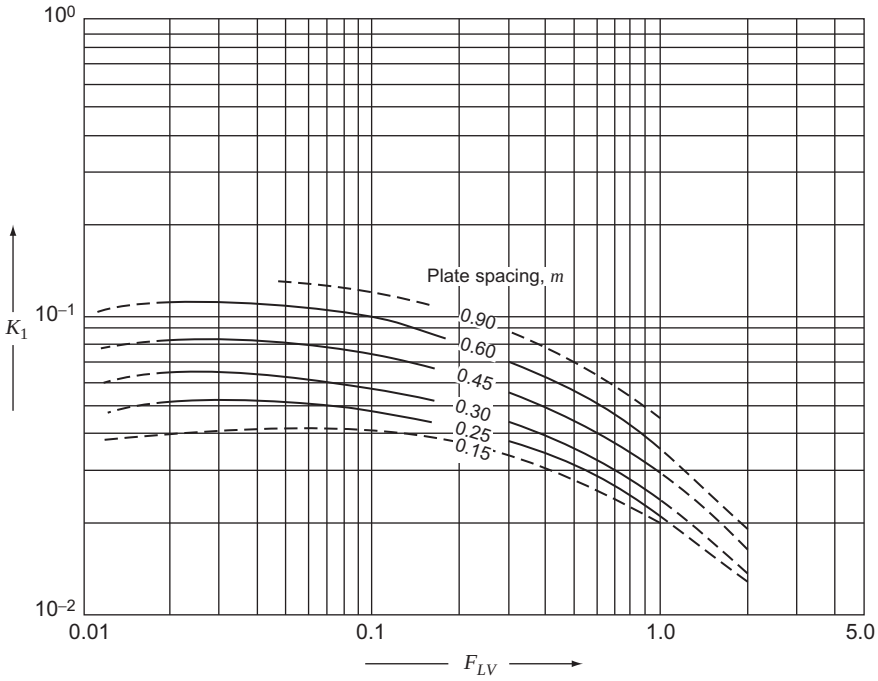


FIG. 17.34 Flooding velocity, sieve plates.

4. Hole: active area ratio greater than 0.10; for other ratios, apply the following corrections:

Hole: active area	Multiply K_1 by
0.10	1.0
0.08	0.9
0.06	0.8

5. Liquid surface tension 0.02 N/m; for other surface tensions, σ, multiply the value of K_1 by $[\sigma/0.02]^{0.2}$

To calculate the column diameter, an estimate of the net area A_n is required. As a first trial take the downcomer area as 12% of the total, and assume that the hole active area is 10%.

Where the vapor and liquid flow rates or physical properties vary significantly throughout the column, a plate design should be made for several points up the column. For distillation, it will usually be sufficient to design for the conditions above and below the feed points. Changes in the vapor flow rate will normally be accommodated by adjusting the hole area, often by blanking off some rows of holes. Different column diameters would only be used where there is a considerable change in flow rate. Changes in liquid rate can be allowed for by adjusting the liquid downcomer areas.

17.13.4 Liquid–flow arrangement

The choice of plate type (reverse, single pass, or multiple pass) will depend on the liquid flow rate and column diameter. An initial selection can be made using Fig. 17.35, which has been adapted from a similar figure given by Huang and Hodson (1958).

17.13.5 Entrainment

Entrainment can be estimated from the correlation given by Fair (1961) (Fig. 17.36), which gives the fractional entrainment ψ (kg/kg gross liquid flow) as a function of the liquid–vapor factor F_{LV}, with the percentage approach to flooding as a parameter.

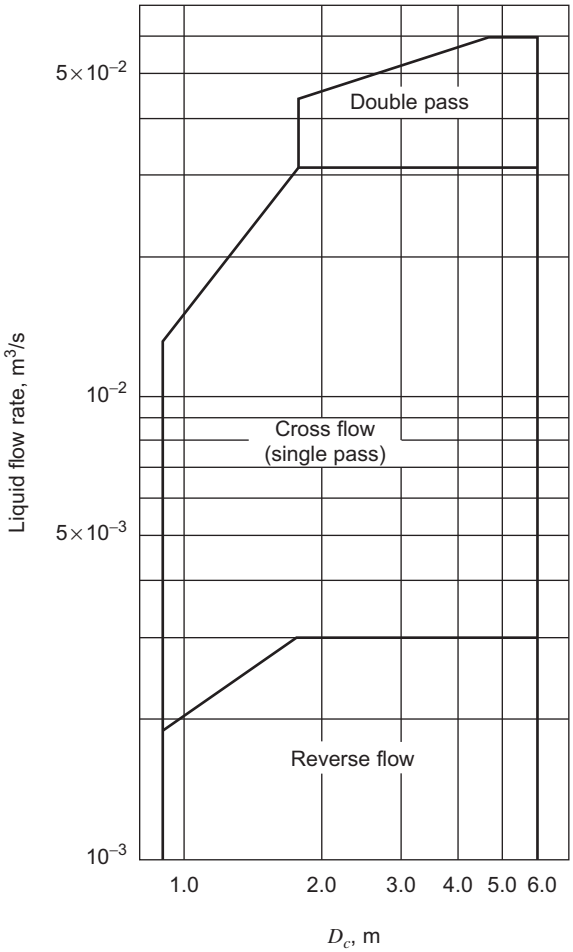


FIG. 17.35 Selection of liquid-flow arrangement.

The percentage flooding is given by:

$$\text{percentage flooding} = \frac{u_n \ (\text{actual velocity based on net area})}{u_f (\text{from Equation 17.49})} \tag{17.51}$$

The effect of entrainment on plate efficiency can be estimated using Equation 17.46.

As a rough guide the upper limit of ψ can be taken as 0.1; below this figure the effect on efficiency will be small. The optimum design value may be above this figure; see Fair (1963).

17.13.6 Weep point

The lower limit of the operating range occurs when liquid leakage through the plate holes becomes excessive. This is known as the weep point. The vapor velocity at the weep point is the minimum value for stable operation. The hole area must be chosen so that at the lowest operating rate the vapor flow velocity is still well above the weep point.

Several correlations have been proposed for predicting the vapor velocity at the weep point; see Chase (1967). That given by Eduljee (1959) is one of the simplest to use and has been shown to be reliable.

The minimum design vapor velocity is given by:

$$u_h = \frac{[K_2 - 0.90(25.4 - d_h)]}{(\rho_v)^{1/2}} \tag{17.52}$$

where u_h = minimum vapor velocity through the holes (based on the hole area), m/s
d_h = hole diameter, mm

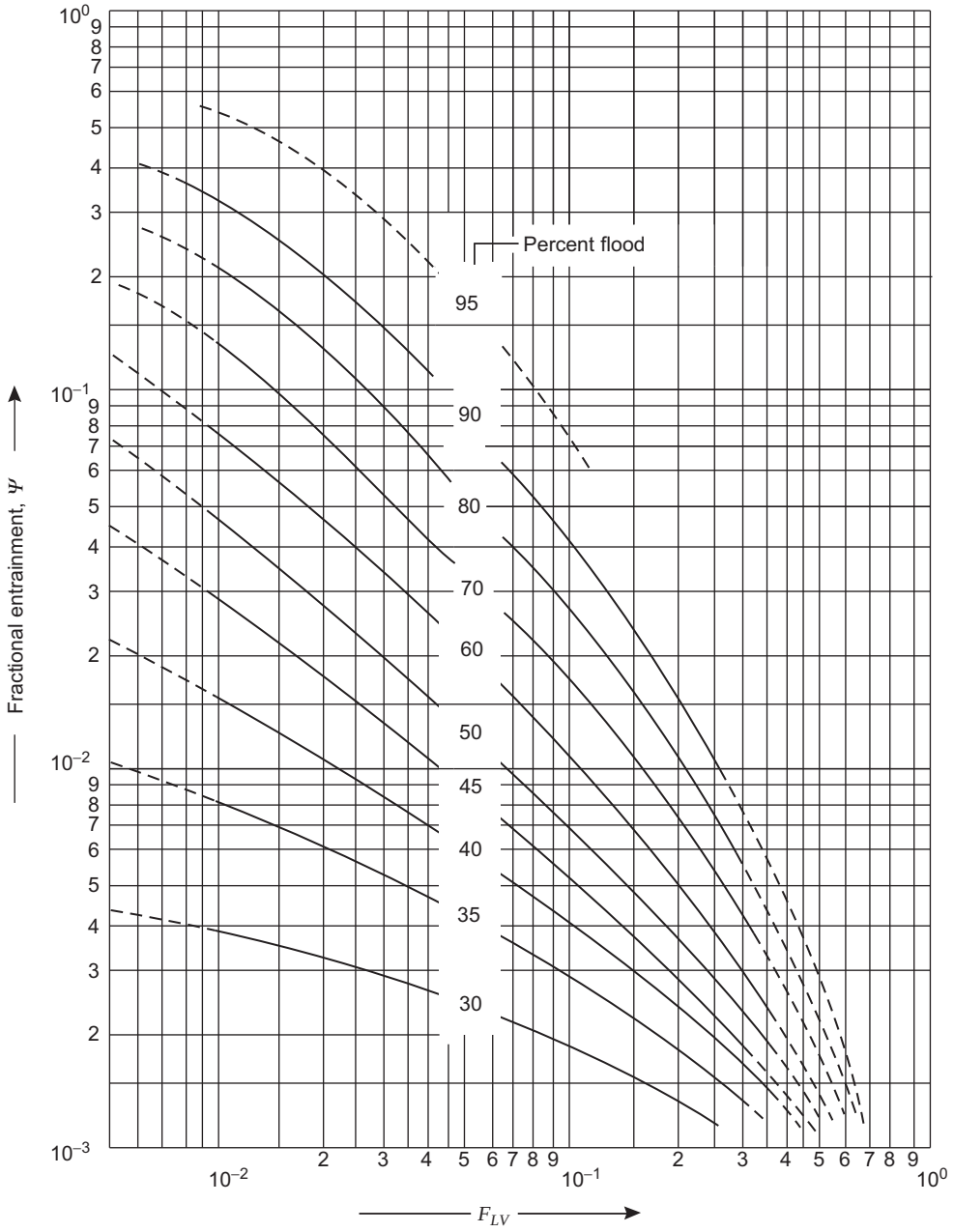


FIG. 17.36 Entrainment correlation for sieve plates. *(From Fair, 1961.)*

K_2 = a constant, dependent on the depth of clear liquid on the plate, obtainedfrom Fig. 17.37

The clear liquid depth is equal to the height of the weir h_w plus the depth of the crest of liquid over the weir h_{ow}; this is discussed in the next section.

17.13.7 Weir liquid crest

The height of the liquid crest over the weir can be estimated using the Francis weir formula (see Chhabra & Shankar, 2017). For a segmental downcomer this can be written as:

$$h_{ow} = 750\left[\frac{L_w}{\rho_L l_w}\right]^{2/3} \tag{17.53}$$

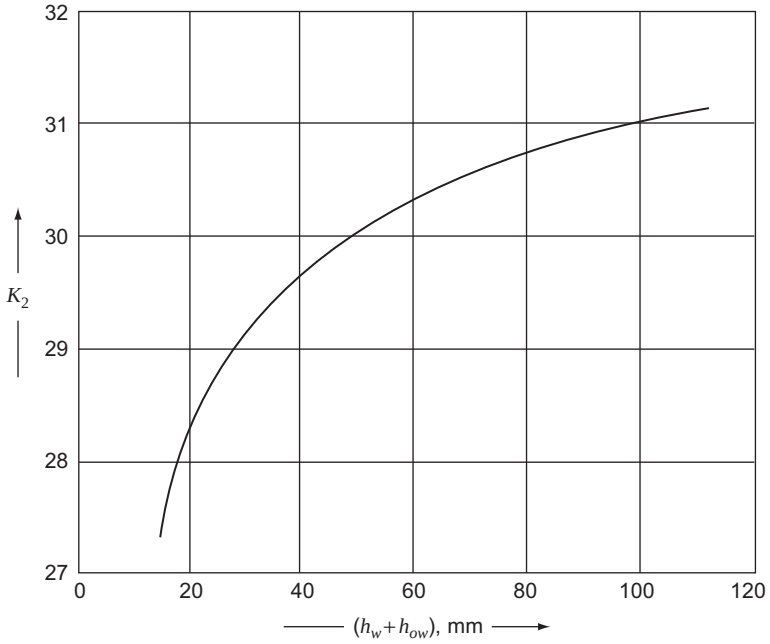


FIG. 17.37 Weep-point correlation. *(From Eduljee, 1959.)*

where l_w = weir length, m
h_{ow} = weir crest, mm liquid
L_w = liquid flow rate, kg/s

With segmental downcomers the column wall constricts the liquid flow, and the weir crest will be higher than that predicted by the Francis formula for flow over an open weir. The constant in Equation 17.53 has been increased to allow for this effect.

To ensure an even flow of liquid along the weir, the crest should be at least 10 mm at the lowest liquid rate. Serrated weirs known as picket-fence weirs are sometimes used for very low liquid rates, as illustrated in Fig. 17.38.

17.13.8 Weir dimensions

Weir height

The height of the weir determines the volume of liquid on the plate and is an important factor in determining the plate efficiency (see Section 17.10.4). A high weir will increase the plate efficiency but at the expense of a higher plate pressure drop. For columns operating above atmospheric pressure, the weir heights will normally be between 40 mm and 90 mm (1.5 and 3.5 in); 40 and 50 mm is recommended. For vacuum operation, lower weir heights are used to reduce the pressure drop; 6 to 12 mm ($\frac{1}{4}$ to $\frac{1}{2}$ in) is recommended.

Inlet weirs

Inlet weirs, or recessed pans, are sometimes used to improve the distribution of liquid across the plate but are seldom needed with segmental downcomers.

Weir length

With segmental downcomers the length of the weir fixes the area of the downcomer. The chord length will normally be between 0.6 and 0.85 of the column diameter. A good initial value to use is 0.77, equivalent to a downcomer

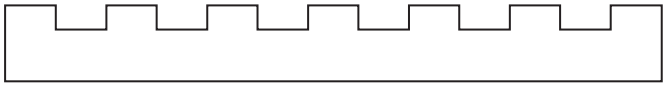


FIG. 17.38 Picket-fence weir.

area of 12%. The liquid flow rate over the weir should ideally be in the range 5 to 8 liters/s per m (2 to 3 gpm/in). If this is not feasible with a single-pass tray, then reverse-flow or multiple-pass trays should be considered, as illustrated in Fig. 17.28. If the liquid flow is too low, then a picket-fence weir can be specified.

The relationship between weir length and downcomer area for segmental downcomers is given in Fig. 17.39.

For double-pass plates, the width of the central downcomer is normally 200 to 250 mm (8 to 10 in).

17.13.9 Perforated area

The area available for perforation will be reduced by the obstruction caused by structural members (the support rings and beams) and by the use of calming zones.

Calming zones are unperforated strips of plate at the inlet and outlet sides of the plate. The width of each zone is usually made the same; recommended values are below 1.5 m diameter, 75 mm; above, 100 mm.

The width of the support ring for sectional plates will normally be 50 to 75 mm: the support ring should not extend into the downcomer area. A strip of unperforated plate will be left around the edge of cartridge-type trays to stiffen the plate.

The unperforated area can be calculated from the plate geometry. The relationship between the weir chord length, the chord height, and the angle subtended by the chord is given in Fig. 17.40.

17.13.10 Hole size

The hole sizes used vary from 2.5 to 19 mm; 5 mm is the preferred size for nonfouling applications. Larger holes are recommended for fouling systems. The holes are drilled or punched. Punching is cheaper, but the minimum size of hole that can be punched will depend on the plate thickness. For carbon steel, hole sizes approximately equal to the plate thickness can be punched, but for stainless steel the minimum hole size that can be punched is about twice the plate thickness. Typical plate thicknesses used are 5 mm ({3/16 }in) for carbon steel and 3 mm (12 gauge) for stainless steel.

When punched plates are used, they should be installed with the direction of punching upward. Punching forms a slight nozzle, and reversing the plate will increase the pressure drop.

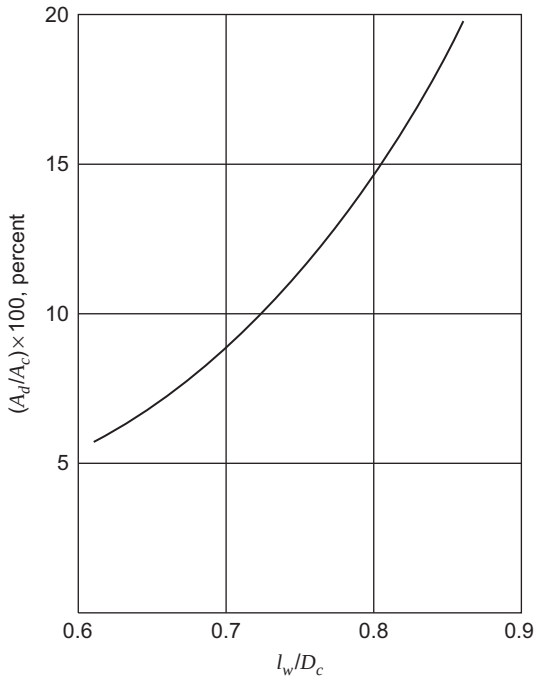


FIG. 17.39 Relation between downcomer area and weir length.

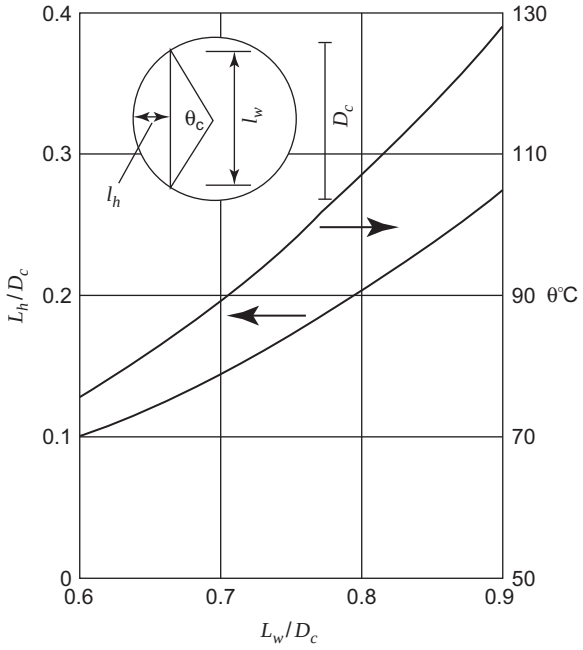


FIG. 17.40 Relation between angle subtended by chord, chord height, and chord length.

17.13.11 Hole pitch

The hole pitch (distance between the hole centers) l_p should not be less than 2.0 hole diameters, and the normal range will be 2.5 to 4.0 diameters. Within this range, the pitch can be selected to give the number of active holes required for the total hole area specified.

Square and equilateral triangular patterns are used; triangular is preferred. The total hole area as a fraction of the perforated area A_p is given by the following expression for an equilateral triangular pitch:

$$\frac{A_h}{A_p} = 0.9\left[\frac{d_h}{l_p}\right]^2 \tag{17.54}$$

This equation is plotted in Fig. 17.41.

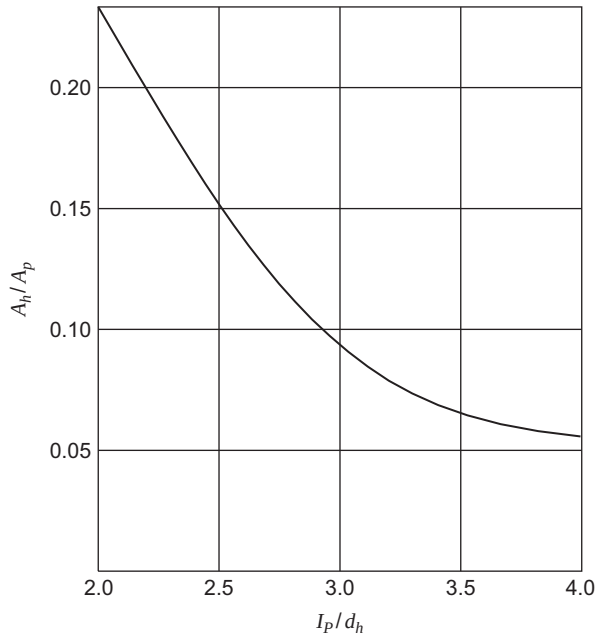


FIG. 17.41 Relation between hole area and pitch.

17.13.12 Hydraulic gradient

The hydraulic gradient is the difference in liquid level needed to drive the liquid flow across the plate. On sieve plates, unlike bubble-cap plates, the resistance to liquid flow will be small, and the hydraulic gradient is usually ignored in sieve-plate design. It can be significant in vacuum operation, as with the low weir heights used, the hydraulic gradient can be a significant fraction of the total liquid depth. Methods for estimating the hydraulic gradient are given by Fair (1963).

17.13.13 Liquid throw

The liquid throw is the horizontal distance traveled by the liquid stream flowing over the downcomer weir. It is only an important consideration in the design of multiple-pass plates. Bolles (1963) gives a method for estimating the liquid throw. If the liquid throw is excessive, antijump baffles can be used to ensure that liquid flows down and does not jump to the adjacent section.

17.13.14 Plate pressure drop

The pressure drop over the plates is an important design consideration. There are two main sources of pressure loss: that due to vapor flow through the holes (an orifice loss) and that due to the static head of liquid on the plate.

A simple additive model is normally used to predict the total pressure drop. The total is taken as the sum of the pressure drop calculated for the flow of vapor through the dry plate (the dry plate drop h_d); the head of clear liquid on the plate ($h_w + h_{ow}$); and a term to account for other, minor, sources of pressure loss, the so-called residual loss h_r. The residual loss is the difference between the observed experimental pressure drop and the simple sum of the dry plate drop and the clear-liquid height. It accounts for the two effects: the energy to form the vapor bubbles and the fact that on an operating plate the liquid head will not be clear liquid but a head of "aerated" liquid froth, and the froth density and height will be different from that of the clear liquid.

It is convenient to express the pressure drops in terms of millimeters of liquid. In pressure units:

$$\Delta P_t = 9.81 \times 10^{-3} h_t \rho_L \tag{17.55}$$

where ΔP_t = total plate pressure drop, Pa (N/m^2)
h_t = total plate pressure drop, mm liquid

Dry plate drop

The pressure drop through the dry plate can be estimated using expressions derived for flow through orifices:

$$h_d = 51 \left[\frac{u_h}{C_0}\right]^2 \frac{\rho_v}{\rho_L} \tag{17.56}$$

where the orifice coefficient C_0 is a function of the plate thickness, hole diameter, and the hole—to—perforated area ratio. C_0 can be obtained from Fig. 17.42, which has been adapted from a similar figure by Liebson et al. (1957). u_h is the velocity through the holes, m/s.

Residual head

Methods have been proposed for estimating the residual head as a function of liquid surface tension, froth density, and froth height; however, as this correction term is small, the use of an elaborate method for its estimation is not justified, and the simple equation proposed by Hunt et al. (1955) can be used:

$$h_r = \frac{12.5 \times 10^3}{\rho_L} \tag{17.57}$$

Equation 17.57 is equivalent to taking the residual drop as a fixed value of 12.5 mm of water ($\frac{1}{2}$ in).

Total drop

The total plate drop is given by:

$$h_t = h_d + (h_w + h_{ow}) + h_r \tag{17.58}$$

If the hydraulic gradient is significant, half its value is added to the clear liquid height.

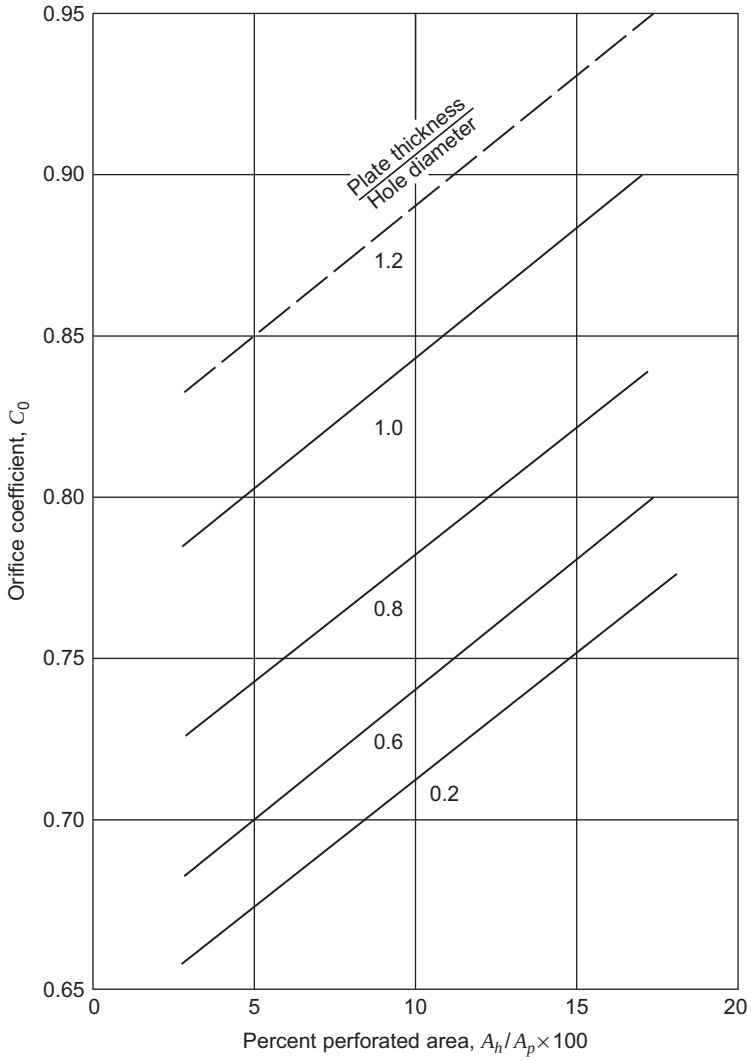


FIG. 17.42 Discharge coefficient, sieve plates. *(From Liebson et al., 1957.)*

17.13.15 Downcomer design (backup)

The downcomer area and plate spacing must be such that the level of the liquid and froth in the downcomer is well below the top of the outlet weir on the plate above. If the level rises above the outlet weir, the column will flood.

The backup of liquid in the downcomer is caused by the pressure drop over the plate (the downcomer in effect forms one leg of a U-tube) and the resistance to flow in the downcomer itself (Fig. 17.43).

In terms of clear liquid, the downcomer backup is given by:

$$h_b = (h_w + h_{ow}) + h_t + h_{dc} \tag{17.59}$$

where h_b = downcomer backup, measured from plate surface, mm
h_{dc} = head loss in the downcomer, mm

The main resistance to flow will be caused by the constriction at the downcomer outlet, and the head loss in the downcomer can be estimated using the equation given by Cicalese et al. (1947):

$$h_{dc} = 166\left[\frac{L_{wd}}{\rho_L A_m}\right]^2 \tag{17.60}$$

where L_{wd} = liquid flow rate in downcomer, kg/s
A_m = either the downcomer area A_d or the clearance area under the downcomer A_{ap}, whichever is smaller, m^2

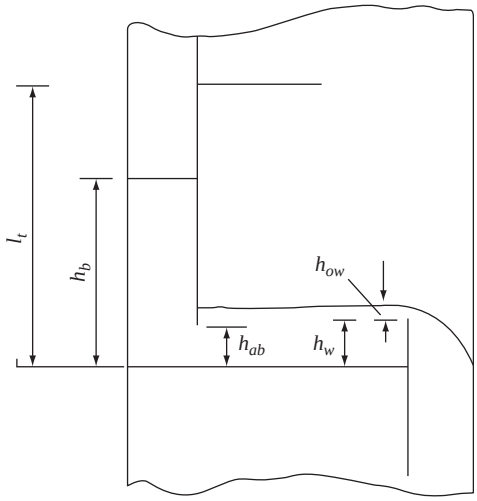


FIG. 17.43 Downcomer back-up.

The clearance area under the downcomer is given by:

$$A_{ap} = h_{ap} l_w \tag{17.61}$$

where h_{ap} is height of the bottom edge of the apron above the plate. This height is normally set at 5 to 10 mm ($\frac{1}{4}$ to $\frac{1}{2}$ in) below the outlet weir height:

$$h_{ap} = h_w - (5 \text{ to } 10 \text{ mm})$$

Froth height

To predict the height of "aerated" liquid on the plate and the height of froth in the downcomer, some means of estimating the froth density is required. The density of the "aerated" liquid will normally be between 0.4 and 0.7 times that of the clear liquid. A number of correlations have been proposed for estimating froth density as a function of the vapor flow rate and the liquid physical properties; see Chase (1967); however, none is particularly reliable, and for design purposes it is usually satisfactory to assume an average value of 0.5 of the liquid density.

This value is also taken as the mean density of the fluid in the downcomer, which means that for safe design the clear liquid backup, calculated from Equation 17.59, should not exceed half the plate spacing l_t, to avoid flooding.

Allowing for the weir height:

$$h_b \leq \tfrac{1}{2}(l_t + h_w) \tag{17.62}$$

This criterion is, if anything, oversafe, and where close plate spacing is desired, a better estimate of the froth density in the downcomer should be made. The method proposed by Thomas and Shah (1964) is recommended. Kister (1992) recommends that the froth height in the downcomer should not be greater than 80% of the tray spacing.

Downcomer residence time

Sufficient residence time must be allowed in the downcomer for the entrained vapor to disengage from the liquid stream, to prevent heavily "aerated" liquid being carried under the downcomer. A time of at least 3 seconds is recommended.

The downcomer residence time is given by:

$$t_r = \frac{A_d h_{bc} \rho_L}{L_{wd}} \tag{17.63}$$

where t_r = residence time, s
h_{bc} = clear liquid backup, m

Example 17.6

Design the plates for the column specified in Example 17.2. Take the minimum feed rate as 70% of the maximum (maximum feed 10,000 kg/h). Use sieve plates.

Solution

As the liquid and vapor flow rates and compositions will vary up the column, plate designs should be made above and below the feed point. Only the bottom plate will be designed in detail in this example.

From the McCabe–Thiele diagram, Example 17.2:

Number of stages = 10
Top composition 95 mol%, bottom composition 1 mol%
Reflux ratio = 1.24

Flow rates

Mol. weight feed $= 0.1 \times 58 + (1-0.1)18 = 22$

Feed $= 10{,}000/22 = 454.5$ kmol/h

Overall mass balance: $D + B = 454.5$

A mass balance on acetone gives:

$$0.95D + 0.01B = 0.1(454.5)$$

Hence: $D = 43.5$ kmol/h, $B = 411.0$ kmol/h

Vapor rate, $V = D(1+R) = 43.5(1+1.24) = 97.5$ kmol/h

The feed is saturated liquid, so:

liquid flow above feed, $L = RD = 1.24(43.52) = 54.0$ kmol/h

liquid flow below feed, $L = RD + F = 454.5 + 54 = 508.5$ kmol/h

Physical properties

Estimate base pressure, assume column efficiency of 60%, ignore reboiler.

$$\text{Number of real stages} = \frac{10}{0.6} = 17$$

Assume pressure drop per plate is 100 mm water.

$$\text{Column pressure drop} = 100 \times 10^{-3} \times 1000 \times 9.81 \times 17 = 16{,}677 \text{ Pa}$$

$$\text{Top pressure, } 1 \text{ atm}\left(14.7 \text{ lb/in}^2\right) = 101.4 \times 10^3 \text{ Pa}$$

$$\text{Estimated bottom pressure} = 101.4 \times 10^3 = 16{,}677$$

$$118{,}077 \text{ Pa} = \underline{\underline{1.18 \text{ bar}}}$$

From UniSim Design, base temperature 96.0 °C:

$$\rho_v = 0.693 \text{ kg/m}^3, \rho_L = 944 \text{ kg/m}^3$$

$$\text{Molecular weight} = 18.4, \text{ surface tension} = 58.9 \times 10^{-3} \text{ N/m}$$

Distillate, 95 mol% acetone, 56 °C:

$$\rho_v = 2.07 \text{ kg/m}^3, \rho_L = 748 \text{ kg/m}^3$$

$$\text{Molecular weight} = 56.1, \text{ surface tension} = 22.7 \times 10^{-3} \text{N/m}$$

Column diameter

Neglecting differences in molecular weight between vapor and liquid:

$$F_{LV}\ \text{bottom} = \frac{508.5}{97.5}\sqrt{\frac{0.693}{944}} = 0.141 \tag{17.50}$$

$$F_{LV}\ \text{top} = \frac{54}{97.5}\sqrt{\frac{2.07}{748}} = 0.0291 \tag{17.50}$$

Take plate spacing as 0.5 m
From Fig. 17.34:

$$\text{base } K_1 = 7.5 \times 10^{-2}$$

$$\text{top } K_1 = 9.0 \times 10^{-2}$$

Correction for surface tensions:

$$\text{base } K_1 = \left(\frac{59}{20}\right)^{0.2} \times 7.5 \times 10^{-2} = 9.3 \times 10^{-2}$$

$$\text{top } K_1 = \left(\frac{23}{20}\right)^{0.2} \times 9.0 \times 10^{-2} = 9.3 \times 10^{-2}$$

$$\text{base } u_f = 9.3 \times 10^{-2}\sqrt{\frac{944 - 0.693}{0.693}} = 3.43\ \text{m/s} \tag{17.49}$$

$$\text{top } u_f = 9.3 \times 10^{-2}\sqrt{\frac{748 - 2.07}{2.07}} = 1.77\ \text{m/s} \tag{17.49}$$

Design for 85% flooding at maximum flow rate:

$$\text{base } u_n = 3.43 \times 0.85 = 2.92\ \text{m/s}$$

$$\text{top } u_n = 1.77 \times 0.85 = 1.50\ \text{m/s}$$

Maximum volumetric flow rate:

$$\text{base} = \frac{97.5 \times 18.4}{0.693 \times 3600} = 0.719\ \text{m}^3/\text{s}$$

$$\text{top} = \frac{97.5 \times 56.1}{2.07 \times 3600} = 0.734\ \text{m}^3/\text{s}$$

Net area required:

$$\text{base} = \frac{0.719}{2.92} = 0.246\ \text{m}^2$$

$$\text{top} = \frac{0.734}{1.50} = 0.489\ \text{m}^2$$

As first trial, take downcomer area as 12% of total:
Column cross-sectioned area:

$$\text{base} = \frac{0.246}{0.88} = 0.280\ \text{m}^2$$

$$\text{top} = \frac{0.489}{0.88} = 0.556\ \text{m}^2$$

Column diameter:

$$\text{base} = \sqrt{\frac{0.28 \times 4}{\pi}} = 0.60\ \text{m}$$

$$\text{top} = \sqrt{\frac{0.556 \times 4}{\pi}} = 0.84\ \text{m}$$

Use same diameter above and below feed, reducing the perforated area for plates above the feed.
This is too large to use standard pipe, so round up to nearest standard head size; inside diameter 914.4 mm (36 in).

Liquid flow pattern

$$\text{Maximum volumetric liquid rate} = \frac{508.5 \times 18.4}{3600 \times 944} = 2.75 \times 10^{-3}\text{m}^3/\text{s}$$

The plate diameter is outside the range of Fig. 17.35, but it is clear that a single-pass plate can be used.

Provisional plate design

Column diameter $D_c = 0.914$ m

Column area $A_c = 0.556$ m^2

Downcomer area $A_d = 0.12 \times 0.556 = 0.067$ m^2, at12%

Net area $A_n = A_c - A_d = 0.556 - 0.067 = 0.489$ m^2

Active area $A_a = A_c - 2A_d = 0.556 - 0.134 = 0.422$ m^2

Hole area A_h take 10% A_a as first trial $= 0.042$ m^2

Weir length (from Fig.17.39) $= 0.76 \times 0.914 = 0.695$ m

Take weir height	50 mm
Hole diameter	5 mm
Plate thickness	5 mm

Check weeping

$$\text{Maximum liquid rate} = \frac{508.5 \times 18.4}{3600} = 2.60 \text{ kg/s}$$

$$\text{Minimum liquid rate at 70\% turndown} = 0.7 \times 2.6 = 1.82 \text{ kg/s}$$

$$\text{Maximum } h_{ow} = \left(\frac{2.6}{944 \times 0.695}\right)^{2/3} = 25.0 \text{ mm liquid} \tag{17.53}$$

$$\text{Minimum } h_{ow} = \left(\frac{1.82}{944 \times 0.695}\right)^{2/3} = 19.7 \text{ mm liquid} \tag{17.53}$$

$$\text{At minimum rate } h_w + h_{ow} = 50 + 19.7 = 69.7 \text{ mm}$$

From Fig. 17.37,

$$K_2 = 30.6$$

$$u_h \text{ (min)} = \frac{[30.6 - 0.90(25.4 - 5)]}{(0.693)^{1/2}} = 14.7 \text{ m/s} \tag{17.52}$$

$$\text{Actual minimum vapor velocity} = \frac{\text{minimum vapour rate}}{A_h} = \frac{0.7 \times 0.719}{0.042} = 12.0 \text{ m/s}$$

So the minimum operating rate will lead to weeping at the bottom of the column. Reduce hole area to 7% of active area $= 0.422 \times 0.07 = 0.0295$ m^2.

$$\text{New actual minimum vapor velocity} = \frac{0.7 \times 0.719}{0.0295} = 17.1 \text{ m/s}$$

which is now well above the weep point.

Plate pressure drop

Dry plate drop:

Maximum vapor velocity through holes:

$$u_h\,(\max) \;=\; \frac{0.719}{0.0295} = \;24.4\ \text{m/s}$$

From Fig. 17.42, for plate thickness/hole diameter = 1 and $A_h/A_p \approx A_h/A_a = 0.07$, $C_0 = 0.82$:

$$h_d \;=\; 51\;\left[\frac{24.4}{0.82}\right]^2\;\frac{0.693}{944} = \;33.1\ \text{mm liquid} \tag{17.56}$$

residual head:

$$h_r \;=\; \frac{12.5\;\times\;10^3}{944} = \;13.2\ \text{mm liquid} \tag{17.55}$$

total plate pressure drop:

$$h_t = 33 + (50{+}\,25) + 13 = 18\ \text{mm liquid}$$

Note: 100 mm was assumed to calculate the base pressure. The calculation could be repeated with a revised estimate, but the small change in physical properties will have little effect on the plate design. 118 mm per plate is considered acceptable.

Downcomer liquid backup

Downcomer pressure loss:

Take $h_{ap} = h_w - 10 = 40$ mm.

Area under apron, $A_{ap} = 0.695 \times 40 \times 10^{-3} = 0.028\text{m}^2$.

As this is less than $A_d = 0.067$, m^2 use A_{ap} in Equation 17.60:

$$h_{dc} \;=\; 166\;\left[\frac{2.60}{944\;\times\;0.028}\right]^2 = \;1.61\ \text{mm} \tag{17.60}$$

say 2 mm.

Backup in downcomer:

$$h_b = (50{+}\,25) + 118 + 2 = 195\ \text{mm} \tag{17.59}$$

$$195\ \text{mm} \;<\; \frac{1}{2}(\text{plate spacing} + \text{weir height}),\ \text{so plate spacing is acceptable}$$

Check residence time:

$$t_r \;=\; \frac{0.067\;\times\;0.195\;\times\;944}{2.60} = \;4.7\ \text{s} \tag{17.63}$$

>3 s, satisfactory.

Check entrainment

$$u_v \;=\; \frac{0.719}{0.489} = \;1.47\ \text{m/s}$$

$$\text{percent flooding} = \frac{1.47}{3.43} = \;42.8\%$$

$$F_{LV} = 0.14,\ \text{so from Fig.17.36,}\ \Psi = 0.0038,\ \text{well below 0.1.}$$

As the percent flooding is well below the design figure of 85, the column diameter could be reduced, but this would increase the pressure drop.

Trial layout

Use cartridge-type construction. Allow 50-mm unperforated strip around plate edge; 50-mm-wide calming zones.

Perforated area

From Fig.17.40, at $l_w/D_c = 0.695/0.914 = 0.76, \theta_c = 99^\circ$

angle subtended by the edge of the plate $= 180 - 99 = 81^\circ$

mean length, unperforated edge strips $= (0.914 - 50 \times 10^{-3})\pi \times 81/180 = 1.22$ m

area of unperforated edge strips $= 50 \times 10^{-3} \times 1.22 = 0.061$ m^2

mean length of calming zone, approx. = weir length + width of unperforated strip

$$= 0.695 + 50 \times 10^{-3} = 0.745 \text{ m}$$

area of calming zones $= 2(0.745 \times 50 \times 10^{-3}) = 0.0745$ m^2

total area for perforations, $A_p = 0.422 - 0.061 - 0.075 = 0.286$ m^2

$A_h/A_p = 0.0295/0.286 = 0.103$

From Fig. 17.41, $l_p/d_h = 2.9$; satisfactory, within 2.5 to 4.0.

Number of holes

$$\text{Area of one hole} = 1.964 \times 10^{-5} \text{m}^2$$

$$\text{Number of holes} = \frac{0.0295}{1.964 \times 10^{-5}} = 1502$$

Plate specification

The final plate specification is shown in Fig. 17.44.

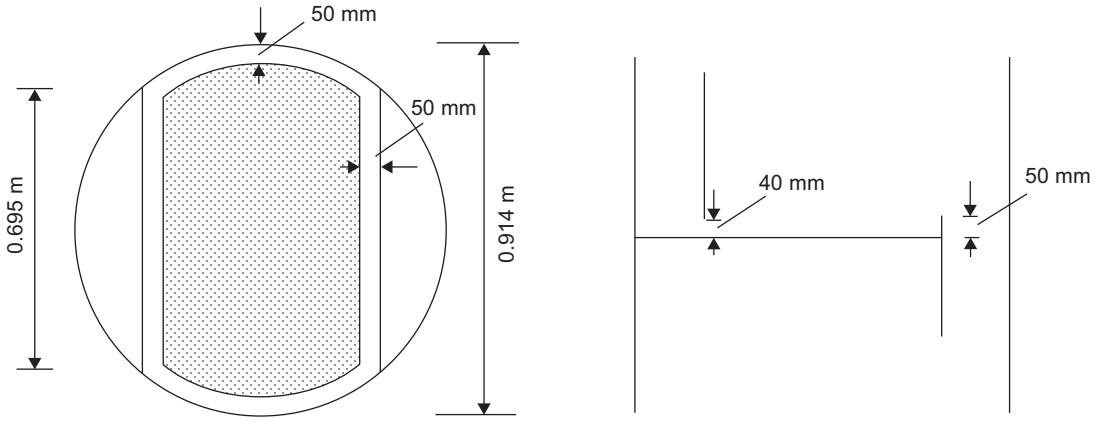


Plate number	1	Turn-down	70% of max rate
Plate inside dia.	0.914 m	Plate material	Mild steel
Hole size	5 mm	Downcomer material	Mild steel
Hole pitch	12.5 mm Δ	Plate spacing	0.5 m
Total holes	-	Plate thickness	5 mm
Active holes	1502	Plate pressure drop	120 mm liquid = 1.1 kPa
Blanking area	-		

FIG. 17.44 Plate specification for Example 17.6.

Example 17.7

For the plate design in Example 17.6, estimate the plate efficiency for the plate on which the concentration of acetone is 5 mol%. Use the AIChE method.

Solution

Plate will be in the stripping section (see Fig. 17.9).
Plate dimensions:

active area $= 0.422\ \text{m}^2$

length between downcomers(Fig.17.40) (liquid path, Z_L) $= 0.914\ (1-2\times 0.175) = 0.594$ m

weir height $= 50$ mm

Flow rates, check efficiency at minimum rates, at column base:

$$\text{Vapor} = 0.7 \times \frac{97.5}{3600} = 0.019\ \text{kmol/s}$$

$$\text{Liquid} = 0.7 \times \frac{508.5}{3600} = 0.099\ \text{kmol/s}$$

From the McCabe–Thiele diagram (Fig. 17.9) at $x = 0.05$, assuming 60% plate efficiency, $y \approx 0.35$. The liquid composition, $x = 0.05$, will occur on around the third plate from the bottom (allowing for the reboiler and 60% efficiency per stage). The pressure on this plate will be approximately:

$$101.4 \times 10^3 + (14 \times 0.118 \times 9.81 \times 944) = 116.7\ \text{kPa}$$

$$\text{say}, 1.17\ \text{bar}$$

At this pressure, the plate temperature will be about 92 °C, and the liquid and vapor physical properties, from UniSim Design are:

Liquid:

$$\text{molar weight} = 20, \rho_L = 932.7\ \text{kg/m}^3, \mu_L = 0.3544 \times 10^{-3}\text{Nm}^{-2}\text{s}, \sigma = 60.2 \times 10^{-3}\text{N/m}$$

Vapor:

$$\text{molar weight} = 32, \rho_v = 1.233\ \text{kg/m}^3, \mu_v = 9.17 \times 10^{-6}\text{Nm}^{-2}\text{s}$$

$$D_L = 4.16 \times 10^{-9}\text{m}^2/\text{s}$$

$$D_v = 17.4 \times 10^{-6}\text{m}^2/\text{s}$$

$$\text{Vapor volumetric flow rate} = \frac{0.019 \times 32}{1.233} = 0.493\ \text{m}^3/\text{s}$$

$$\text{Liquid volumetric flow rate} = \frac{0.099 \times 20}{932.7} = 2.12 \times 10^{-3}\text{m}^3/\text{s}$$

$$u_a = \frac{0.493}{0.422} = 1.17\ \text{m/s}$$

$$F_v = u_a \sqrt{\rho_v} = 2.365\ \text{kg}^{0.5}\text{m}^{-0.5}\text{s}^{-1}$$

Average width over active surface $= 0.422/0.594 = 0.71$ m

$$L_p = \frac{2.12 \times 10^{-3}}{0.71} = 2.99 \times 10^{-3} \text{m}^2/\text{s}$$

$$N_G = \frac{\left(0.776 + 4.57 \times 10^{-3} \times 50 - 0.24 \times 2.365 + 105 \times 2.99 \times 10^{-3}\right)}{\left(\frac{9.17 \times 10^{-6}}{1.233 \times 17.4 \times 10^{-6}}\right)^{0.5}} = 1.15 \quad (17.38)$$

$$Z_c = 0.006 + 0.73 \times 10^{-3} \times 50 - 0.24 \times 10^{-3} \times 2.365 \times 50 + 1.22 \times 2.99 \times 10^{-3} \quad (17.43)$$
$$= 17.8 \times 10^{-3}$$

$$t_L = \frac{17.8 \times 10^{-3} \times 0.594}{2.99 \times 10^{-3}} = 3.54 \text{ s} \quad (17.41)$$

$$\mathbf{N}_L = \left(4.13 \times 10^8 \times 4.16 \times 10^{-9}\right)^{0.5} (0.21 \times 2.365 + 0.15) \times 3.54 = 3.00 \quad (17.40)$$

$$D_e = \left(0.0038 + 0.017 \times 1.17 + 3.86 \times 2.99 + 10^{-3} + 0.18 \times 10^{-3} \times 50\right)^2 \quad (17.45)$$
$$= 1.96 \times 10^{-3}$$

$$\text{Pe} = \frac{(0.594)^2}{1.96 \times 10^{-3} \times 3.54} = 50.8 \quad (17.44)$$

From the McCabe–Thiele diagram, at $x = 0.05$, the slope of the equilibrium line ≈ 12.0, so:

$$\frac{m\,V}{L} = \frac{12 \times 0.019}{0.099} = 2.30$$

$$\frac{\left(\frac{m\,V}{L}\right)}{\mathbf{N}_L} = \frac{2.30}{3.00} = 0.767$$

From Fig. 17.21, $E_{mv} = 0.43$:

$$\frac{m\,V}{L} \times E_{mv} = 2.30 \times 43 = 0.989$$

From Fig. 17.22, $E_{mV}/E_{mv} = 1.62$:

$$E_{mV} = 0.43 \times 1.62 = 0.697$$

So plate efficiency $= 70\%$.

Note: The slope of the equilibrium line is difficult to determine at $x = 0.05$, but any error will not greatly affect the value of E_{mV}.

Example 17.8

Calculate the plate efficiency for the plate design considered in Examples 17.6 and 17.7, using Van Winkle's correlation.

Solution

From Examples 17.6 and 17.7:

$$\rho_L = 932.7 \text{ kg/m}^3, \mu_L = 0.3544 \times 10^{-3}\text{Nm}^{-2}\text{s}, D_{LK} = D_L = 4.16 \times 10^{-9}\text{m}^2/\text{s}, \sigma = 60.2 \times 10^{-3} \text{ N/m}$$

$$\rho_v = 1.233 \text{ kg/m}^3, \mu_v = 9.17 \times 10^{-6}\text{Nm}^{-2}\text{s}$$

$$h_w = 50 \text{ mm}$$

$$FA(\text{fractional area}) = A_h/A_c = 0.0295/0.556 = 0.053$$

$$u_v = \text{superficial vapor velocity} = 0.493/0.556 = 0.887 \text{ m/s}$$

$$\text{Dg} = \left(\frac{0.0602}{0.3544 \times 10^{-3} \times 0.887}\right) = 191.6$$

$$\text{Sc} = \left(\frac{0.3544 \times 10^{-3}}{932.7 \times 4.16 \times 10^{-9}}\right) = 91.3$$

$$\text{Re} = \left(\frac{50 \times 10^{-3} \times 0.887 \times 932.7}{0.3544 \times 0.053}\right) = 2.2 \times 10^3$$

$$E_{mV} = 0.07(191.6)^{0.14}(91.3)^{0.25}\left(2.2 \times 10^3\right)^{0.08}$$
$$= \underline{\underline{0.836}} \ (84\%) \qquad (17.36)$$

This seems rather large compared with the value found using the AIChE method, so the value calculated in Example 17.7 is preferred.

17.14 Packed columns

Packed columns are used for distillation, gas absorption, and liquid–liquid extraction; only distillation and absorption will be considered in this section. Stripping (desorption) is the reverse of absorption and the same design methods apply.

The gas–liquid contact in a packed column is continuous, not stage-wise like a plate column. The liquid flows down the column over the packing surface, and the gas or vapor flows countercurrently, up the column. In some gas absorption columns co-current flow is used. The performance of a packed column is highly dependent on the maintenance of good liquid and gas distribution throughout the packed bed, and this is an important consideration in packed-column design.

A schematic diagram, showing the main features of a packed absorption column, is given in Fig. 17.45. A packed distillation column will be similar to the plate columns shown in Fig. 17.1, with the plates replaced by packed sections.

The design of packed columns using random packings is covered in books by Kister (1992), Strigle (1994), and Billet (1995).

Choice of plates or packing

The choice between a plate or packed column for a particular application can only be made with complete assurance by costing each design; however, the choice can usually be made on the basis of experience by considering the main advantages and disadvantages of each type, listed here:

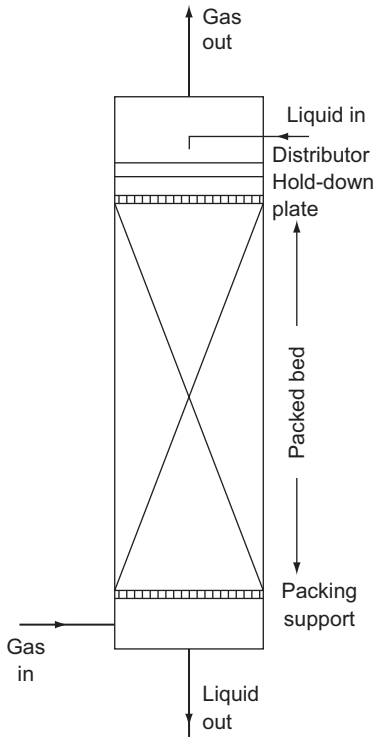


FIG. 17.45 Packed absorption column.

1. Plate columns can be designed to handle a wider range of liquid and gas flow rates than packed columns.
2. Packed columns are not suitable for very low liquid rates.
3. The efficiency of a plate can be predicted with more certainty than the equivalent term for packing (HETP or HTU).
4. Plate columns can be designed with more assurance than packed columns. There is always some doubt that good liquid distribution can be maintained throughout a packed column under all operating conditions, particularly in large columns.
5. It is easier to make provision for cooling in a plate column; coils can be installed on the plates.
6. It is easier to make provision for the withdrawal of side streams from plate columns.
7. If the liquid causes fouling or contains solids, it is easier to make provision for cleaning in a plate column; manways can be installed on the plates. With small-diameter columns, it may be cheaper to use packing and replace the packing when it becomes fouled.
8. For corrosive liquids, a packed column will usually be cheaper than the equivalent plate column.
9. The liquid hold-up is appreciably lower in a packed column than a plate column. This can be important when the inventory of toxic or flammable liquids must be minimized for safety reasons.
10. Packed columns are more suitable for handling foaming systems.
11. The pressure drop per equilibrium stage (HETP) can be lower for packing than plates, and packing should be considered for vacuum columns.
12. Packing should always be considered for small-diameter columns, say less than 0.6 m, where plates would be difficult to install and expensive.

Packed-column design procedures

The design of a packed column involves the following steps:

1. Select the type and size of packing.
2. Determine the column height required for the specified separation.
3. Determine the column diameter (capacity) to handle the liquid and vapor flow rates.
4. Select and design the column internal features: packing support, liquid distributor, redistributors.

These steps are discussed in the following sections, and a packed-column design is illustrated in Example 17.9.

17.14.1 Types of packing

The principal requirements of a packing are that it should:

Provide a large surface area: a high interfacial area between the gas and liquid.
Have an open structure: low resistance to gas flow.
Promote uniform liquid distribution on the packing surface.
Promote uniform vapor or gas flow across the column cross-section.

Many types and shapes of packing have been developed to satisfy these requirements. They can be divided into two broad classes:

1. Packings with a regular geometry, such as stacked rings, grids, and proprietary structured packings.
2. Random packings: rings, saddles, and proprietary shapes, which are dumped into the column and take up a random arrangement.

Grids have an open structure and are used for high gas rates, where low pressure drop is essential; for example, in cooling towers. Random packings and structured packing elements are more commonly used in the process industries.

Random packing

The principal types of random packings are shown in Fig. 17.46. Design data for these packings are given in Table 17.2. The design methods and data given in this section can be used for the preliminary design of packed columns, but for detailed design, it is advisable to consult the packing manufacturer's technical literature to obtain data for the particular packing that will be used. The packing manufacturers should be consulted for details of the many special types of packing that are available for special applications.

Raschig rings (Fig. 17.46a) are one of the oldest specially manufactured types of random packing and are still in general use. Pall rings (see Fig. 17.46b) are essentially Raschig rings in which openings have been made by folding strips of the surface into the ring. This increases the free area and improves the liquid distribution characteristics. Berl saddles (see Fig. 17.46c) were developed to give improved liquid distribution compared with Raschig rings. INTALOX saddles (see Fig. 17.46d) can be considered to be an improved type of Berl saddle; their shape makes them easier to manufacture than Berl saddles. The HY-PAK and SUPER INTALOX packings shown in Fig. 17.46(e and f) can be considered improved types of Pall ring and INTALOX saddle, respectively.

INTALOX saddles, SUPER INTALOX, and HY-PAK packings are proprietary designs and registered trademarks of Koch-Glitsch, LP.

Ring and saddle packings are available in a variety of materials: ceramics, metals, plastics, and carbon. Metal and plastics (polypropylene) rings are more efficient than ceramic rings, as it is possible to make the walls thinner.

Raschig rings are cheaper per unit volume than Pall rings or saddles but are less efficient, and the total cost of the column will usually be higher if Raschig rings are specified. For new columns, the choice will normally be between Pall rings and Berl or INTALOX saddles.

The choice of material will depend on the nature of the fluids and the operating temperature. Ceramic packing will be the first choice for corrosive liquids, but ceramics are unsuitable for use with strong alkalis. Packings made of plastics are attacked by some organic solvents and can only be used up to moderate temperatures, so are unsuitable for distillation columns. Where the column operation is likely to be unstable, metal rings should be specified, as ceramic packing is easily broken. The choice of packings for distillation and absorption is discussed in detail by Eckert (1963), Strigle (1994), Kister (1992), and Billet (1995).

Packing size

In general, the largest size of packing that is suitable for the size of column should be used, up to 50 mm. Small sizes are appreciably more expensive than the larger sizes.

Above 50 mm, the lower cost per cubic meter does not normally compensate for the lower mass transfer efficiency. Use of too large a size in a small column can cause poor liquid distribution.

Recommended size ranges are:

Column diameter	Use packing size
<0.3 m (1 ft)	<25 mm (1 in)
0.3 to 0.9 m (1 to 3 ft)	25 to 38 mm (1 to 1.5 in)
>0.9 m	50 to 75 mm (2 to 3 in)

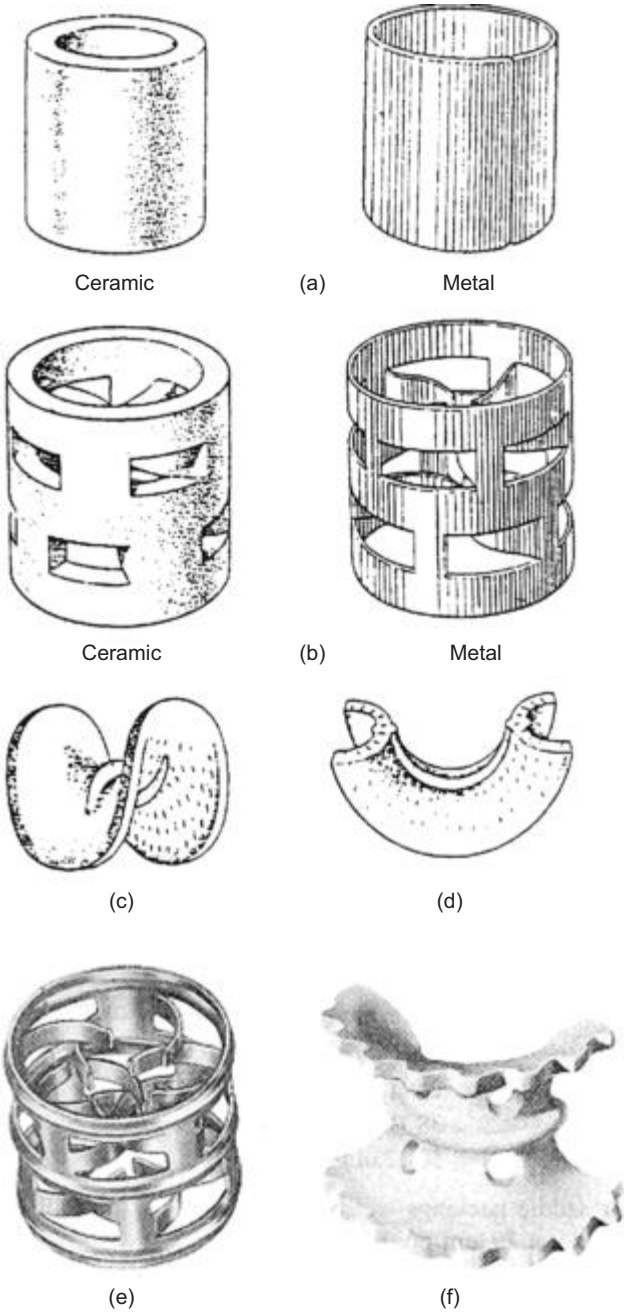


FIG. 17.46 Types of packing (Koch-Glitsch, LP). (a) Raschig rings. (b) Pall rings. (c) Berl saddle ceramic. (d) INTALOX saddle ceramic. (e) Metal HY-PAK. (f) Ceramic, SUPER INTALOX.

Structured packing

The term *structured packing* refers to packing elements made up from wire mesh or perforated metal sheets. The material is folded and arranged with a regular geometry to give a high surface area with a high void fraction. A typical example is shown in Fig. 17.47.

Different designs of structured packing are produced by a number of manufacturers. The basic construction and performance of the various proprietary types available are similar. They are available in metal, plastics, and stoneware. The advantage of structured packing over random packing is their low HETP (typically less than 0.5 m) and low pressure drop (around 100 Pa/m). They are being increasingly used in the following applications:

TABLE 17.2 Design data for various packings

	Size				
	in.	**mm**	**Bulk density (kg/m^3)**	**Surface area a (m^2/m^3)**	**Packing factor F_pm^{-1}**
Raschig rings ceramic	0.50	13	881	368	2100
	1.0	25	673	190	525
	1.5	38	689	128	310
	2.0	51	651	95	210
	3.0	76	561	69	120
Metal (density for carbon steel)	0.5	13	1201	417	980
	1.0	25	625	207	375
	1.5	38	785	141	270
	2.0	51	593	102	190
	3.0	76	400	72	105
Pall rings metal (density for carbon steel)	0.625	16	593	341	230
	1.0	25	481	210	160
	1.25	32	385	128	92
	2.0	51	353	102	66
	3.5	76	273	66	52
Plastics (density for polypropylene)	0.625	16	112	341	320
	1.0	25	88	207	170
	1.5	38	76	128	130
	2.0	51	68	102	82
	3.5	89	64	85	52
INTALOX saddles ceramic	0.5	13	737	480	660
	1.0	25	673	253	300
	1.5	38	625	194	170
	2.0	51	609	108	130
	3.0	76	577		72

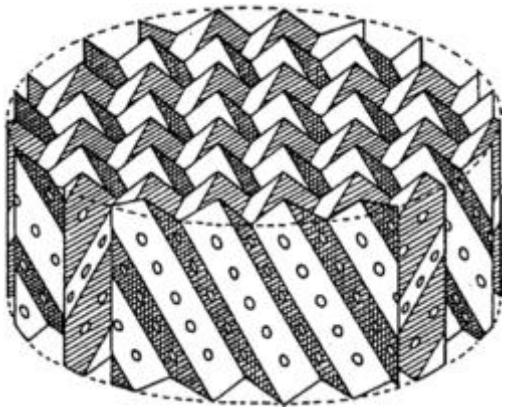


FIG. 17.47 Make-up of structured packing. *(Reproduced from Butcher [1988] with permission.)*

1. For difficult separations, requiring many stages, such as the separation of isomers.
2. High vacuum distillation.
3. For column revamps, to increase capacity and reduce reflux ratio requirements.

The applications have mainly been in distillation, but structured packing can also be used in absorption, in applications where high efficiency and low pressure drop are needed.

The cost of structured packing per cubic meter will be significantly higher than that of random packing, but this is offset by their higher efficiency.

The manufacturers' technical literature should be consulted for design data. A review of the types available is given by Butcher (1988). Generalized methods for predicting the capacity and pressure drop of structured packing are given by Fair and Bravo (1990) and Kister and Gill (1992). The use of structured packing in distillation is discussed in detail in the book by Kister (1992).

Structured packing has a high surface area of thin metal and consequently can be susceptible to ignition of trapped hydrocarbons or pyrophoric corrosion products, as heat is not easily conducted away from local hot spots. The FRI Design Practices Committee has provided guidelines on the design and maintenance of packed columns to reduce the likelihood of packing fires; see FRI Design Practices Committee (2007).

17.14.2 Packed-bed height

Distillation

For the design of packed distillation columns, it is simpler to treat the separation as a staged process and use the concept of the height of an equivalent equilibrium stage to convert the number of ideal stages required to a height of packing. The methods for estimating the number of ideal stages given in Sections 17.5 to 17.8 can then be applied to packed columns.

The height of an equivalent equilibrium stage, usually called the height equivalent to a theoretical plate (HETP), is the height of packing that will give the same separation as an equilibrium stage. It has been shown by Eckert (1975) that in distillation, the HETP for a given type and size of packing is essentially constant and independent of the system physical properties, providing good liquid distribution is maintained and the pressure drop is at least above 17 mm water per meter of packing height. The following values for Pall rings can be used to make an approximate estimate of the bed height required:

Size, mm	HETP, m
25 (1 in)	0.4–0.5
38 (1 $\frac{1}{2}$ in)	0.6–0.75
50 (2 in)	0.75–1.0

The HETP for saddle packings will be similar to that for Pall rings, providing the pressure drop is at least 29 mm per m.

The HETP for Raschig rings will be higher than for Pall rings or saddles, and the values given earlier will only apply at an appreciably higher pressure drop, greater than 42 mm per m.

The methods for estimating the heights of transfer units (HTU), given in Section 17.14.3, can be used for distillation. The relationship between transfer units and the HETP is given by:

$$\text{HETP} = \frac{\mathbf{H}_{OG} \ln\left(\dfrac{mG_m}{L_m}\right)}{\left(\dfrac{mG_m}{L_m} - 1\right)} \tag{17.64}$$

where $\mathbf{H}_{OG}$ is the height of an overall gas-phase transfer unit.

The slope of the equilibrium line m will normally vary throughout a distillation column, so it will be necessary to calculate the HETP for each plate or a series of plates.

Absorption

Though packed absorption and stripping columns can also be designed as staged processes, it is usually more convenient to use the integrated form of the differential equations set up by considering the rates of mass transfer at a point in the column. The derivation of these equations is given in Chhabra and Gurappa (2019).

Where the concentration of the solute is small, say less than 10%, the flow of gas and liquid will be essentially constant throughout the column, and the height of packing required, Z, is given by:

$$Z = \frac{G_m}{K_G a P} \int_{y_2}^{y_1} \frac{dy}{y - y_e} \tag{17.65}$$

in terms of the overall gas-phase mass transfer coefficient K_G and the gas composition.

Or,

$$Z = \frac{L_m}{K_L a C_t} \int_{x_2}^{x_1} \frac{dx}{x_e - x} \tag{17.66}$$

in terms of the overall liquid-phase mass transfer coefficient K_L and the liquid composition,

where G_m = molar gas flow rate per unit cross-sectional area
L_m = molar liquid flow rate per unit cross-sectional area
a = interfacial surface area per unit volume
P = total pressure
C_t = total molar concentration
y_1 and y_2 = the mol fractions of the solute in the gas at the bottom and top of the column, respectively
x_1 and x_2 = the mol fractions of the solute in the liquid at the bottom and top of the column, respectively
x_e = the mole fraction in the liquid that would be in equilibrium with the gas concentration at any point
y_e = the mole fraction in the gas that would be in equilibrium with the liquid concentration at any point

The relationship between the equilibrium concentrations and actual concentrations is shown in Fig. 17.48.

For design purposes, it is convenient to write Equations 17.65 and 17.66 in terms of "transfer units" (HTU); where the value of the integral is the number of transfer units and the group in front of the integral sign, which has units of length, is the height of a transfer unit.

$$Z = \mathbf{H}_{OG}\mathbf{N}_{OG} \tag{17.67a}$$

or

$$Z = \mathbf{H}_{OL}\mathbf{N}_{OL} \tag{17.67b}$$

where $\mathbf{H}_{OG}$ is the height of an overall gas-phase transfer unit:

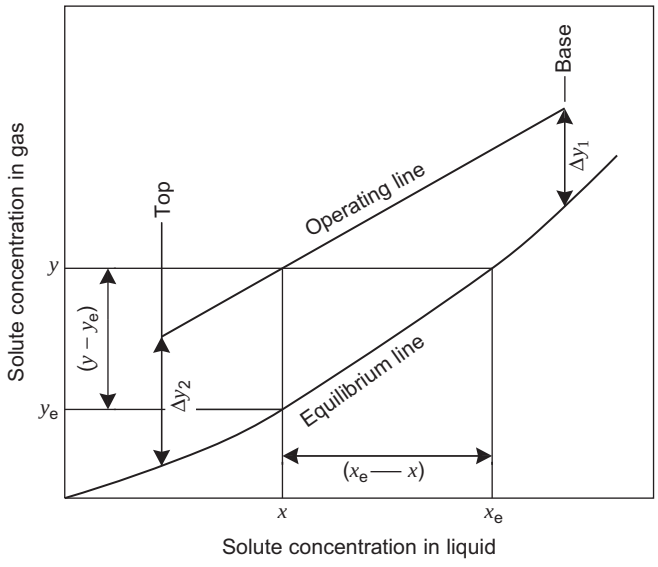


FIG. 17.48 Gas absorption concentration relationships.

$$= \frac{G_m}{K_G a P} \tag{17.68}$$

$\mathbf{N}_{OG}$ is the number of overall gas-phase transfer units:

$$= \int_{y_2}^{y_1} \frac{dy}{y - y_e} \tag{17.69}$$

$\mathbf{H}_{OL}$ is the height of an overall liquid-phase transfer unit:

$$= \frac{L_m}{K_L a C_t} \tag{17.70}$$

$\mathbf{N}_{OL}$ is the number of overall liquid-phase transfer units:

$$= \int_{x_2}^{x_1} \frac{dx}{x_e - x} \tag{17.71}$$

The number of overall gas-phase transfer units is often more conveniently expressed in terms of the partial pressure of the solute gas.

$$\mathbf{N}_{OG} = \int_{p_1}^{p_2} \frac{dp}{p - p_e} \tag{17.72}$$

The relationship between the overall height of a transfer unit and the individual film transfer units $\mathbf{H}_L$ and $\mathbf{H}_G$, which are based on the concentration driving force across the liquid and gas films, is given by:

$$\mathbf{H}_{OG} = \mathbf{H}_G + m\frac{G_m}{L_m}\mathbf{H}_L \tag{17.73}$$

$$\mathbf{H}_{OL} = \mathbf{H}_L + \frac{L_m}{m\, G_m}\mathbf{H}_G \tag{17.74}$$

where m is the slope of the equilibrium line and G_m/L_m the slope of the operating line.

The number of transfer units is obtained by graphical or numerical integration of Equations 17.69, 17.71, or 17.72.

Where the operating and equilibrium lines are straight, and they can usually be considered to be so for dilute systems, the number of transfer units is given by:

$$\mathbf{N}_{OG} = \frac{y_1 - y_2}{\Delta y_{1\mathrm{m}}} \tag{17.75}$$

where Δy_{lm} is the log mean driving force, given by:

$$y_{1\mathrm{m}} = \frac{\Delta y_1 - \Delta y_2}{\ln\left(\frac{\Delta y_1}{\Delta y_2}\right)} \tag{17.76}$$

where $\Delta y_1 = y_1 - y_e$
$\Delta y_2 = y_2 - y_e$

If the equilibrium curve and operating lines can be taken as straight and the solvent feed is essentially solute free, the number of transfer units is given by:

$$\mathbf{N}_{OG} = \frac{1}{1 - \left(\frac{mG_m}{L_m}\right)} \ln\left[\left(1 - \frac{mG_m}{L_m}\right)\frac{y_1}{y_2} + \frac{mG_m}{L_m}\right] \tag{17.77}$$

This equation is plotted in Fig. 17.49, which can be used to make a quick estimate of the number of transfer units required for a given separation.

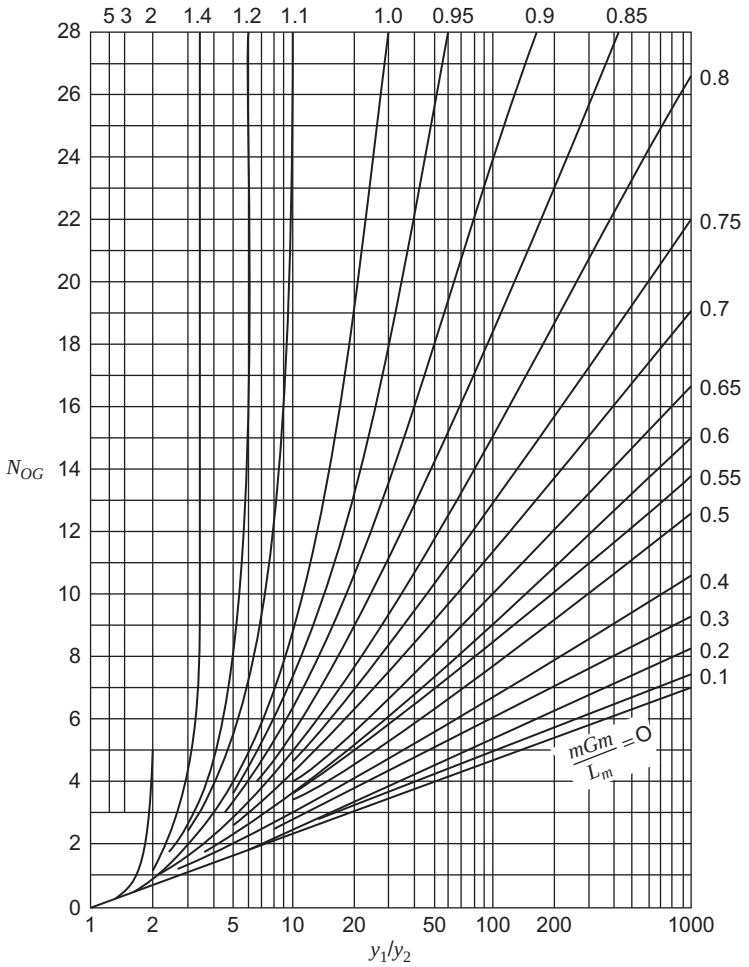


FIG. 17.49 Number of transfer units $\mathbf{N}_{OG}$ as a function of y_1/y_2 with mG_m/L_m as parameter.

It can be seen from Fig. 17.49 that the number of stages required for a given separation is highly dependent on the flow rate L_m. If the solvent rate is not set by other process considerations, Fig. 17.49 can be used to make quick estimates of the column height at different flow rates to find the most economic value. Colburn (1939) has suggested that the optimum value for the term mG_m/L_m will lie between 0.7 and 0.8.

Only physical absorption from dilute gases has been considered in this section. For a discussion of absorption from concentrated gases and absorption with chemical reaction, the reader should refer to Chhabra and Gurappa (2019) or to the book by Treybal (1980). The special case of absorption of acid gases is discussed extensively in the book by Kohl and Nielsen (1997). If the inlet gas concentration is not too high, the equations for dilute systems can be used by dividing the operating line up into two or three straight sections.

Stripping

In a stripping column, an absorbed solute is removed from a liquid solvent by countercurrent contact with a vapor. Stripping and absorption are usually used together, with a stripping column regenerating the solvent for an absorber column. The analysis of stripping is similar to that for absorption; see Green and Southard (2018).

Because the objective in stripping is to achieve a desired outlet liquid concentration, it is more customary to work in overall liquid-phase transfer units:

$$\mathbf{N}_{OL} = \int_{x_2}^{x_1} \frac{\mathrm{d}x}{x_e - x} \tag{17.71}$$

If the equilibrium and operating lines can be taken as straight and the stripping vapor is essentially solute free, the number of transfer units is given by:

$$\mathbf{N}_{OL} = \frac{1}{\left(1 - \frac{L}{mG}\right)} \ln\left[\left(\frac{L}{mG}\right) + \left(1 - \frac{L}{mG}\right)\frac{x_2}{x_1}\right] \tag{17.78}$$

The parameter (L/mG) is known as the stripping factor.

When there are strong chemical interactions between the solute and solvent, the effect is usually to make the equilibrium line curve so that it is concave upwards, as shown in Fig. 17.50. The operating line for stripping must lie below the equilibrium line, so if a low outlet concentration of solute is needed, as is often the case, then L/G must be less than the slope of the equilibrium line, m.

To achieve $L/G < m$, the designer can raise the stripping vapor rate, G, or increase temperature or reduce pressure to increase m.

As the equilibrium line becomes more concave, it obviously becomes more difficult to achieve $L/G < m$ and obtain completely regenerated solvent. Absorber–stripper processes are therefore used for bulk separations, as it is too expensive to completely regenerate the solvent. If necessary, residual amounts of solute in the vapor leaving the absorber can be recovered using adsorption; see Section 16.2.1.

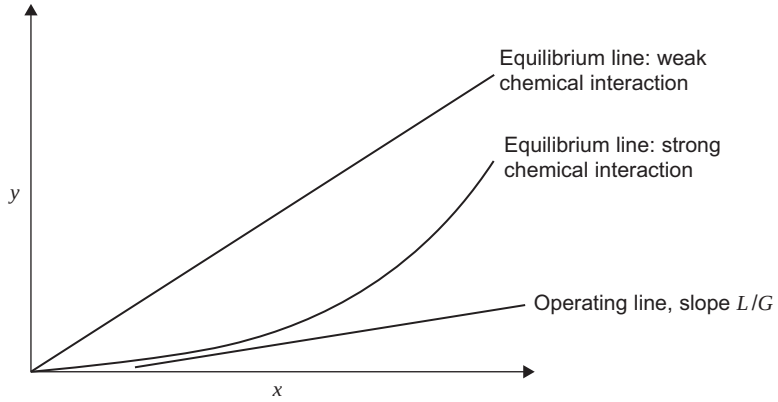


FIG. 17.50 Equilibrium and operating lines for stripping.

17.14.3 Prediction of the height of a transfer unit

There is no entirely satisfactory method for predicting the height of a transfer unit. In practice, the value for a particular packing will depend not only on the physical properties and flow rates of the gas and liquid but also on the uniformity of the liquid distribution throughout the column, which is dependent on the column height and diameter. This makes it difficult to extrapolate data obtained from small-size laboratory and pilot plant columns to industrial-scale columns. Whenever possible, estimates should be based on actual values obtained from operating columns of similar size to that being designed.

Experimental values for several systems are given by Cornell et al. (1960), Eckert (1963), and Vital et al. (1984). A selection of values for a range of systems is given in Table 17.3. The composite mass transfer term $K_G a$ is normally used when reporting experimental mass transfer coefficients for packing, as the effective interfacial area for mass transfer will be less than the actual surface area a of the packing.

Many correlations have been published for predicting the height of a transfer unit and the mass transfer coefficients; several are reviewed in Chhabra and Gurappa (2019). The two methods given in this section have been found to be reliable for preliminary design work and, in the absence of practical values, can be used for the final design with a suitable factor of safety.

The approach taken by the authors of the two methods is fundamentally different, and this provides a useful cross-check on the predicted values. Judgment must always be used when using predictive methods in design, and it is always worthwhile trying several methods and comparing the results.

TABLE 17.3 Typical packing efficiencies

System	Pressure kPa	Column dia, m	Packing Type	Packing Size, mm	HTU m	HETP m
Absorption						
Hydrocarbons	6000	0.9	Pall	50		0.85
NH_3–Air–H_2O	101	—	Berl	50	0.50	
Air–water	101	—	Berl	50	0.50	
Acetone–water	101	0.6	Pall	50		0.75
Distillation						
Pentane–propane	101	0.46	Pall	25		0.46
IPA–water	101	0.46	Int.	25	0.75	0.50
Methanol–water	101	0.41	Pall	25	0.52	
	101	0.20	Int.	25		0.46
Acetone–water	101	0.46	Pall	25		0.37
	101	0.36	Int.	25		0.46
Formic acid–water	101	0.91	Pall	50		0.45
Acetone–water	101	0.38	Pall	38	0.55	0.45
	101	0.38	Int.	50	0.50	0.45
	101	1.07	Int.	38		1.22
MEK–toluene	101	0.38	Pall	25	0.29	0.35
	101	0.38	Int.	25	0.27	0.23
	101	0.38	Berl	25	0.31	0.31

Pall = Pall rings, Berl = Berl saddles, Int. = INTALOX saddles.

Typical values for the HTU of random packings are:

25 mm (1 in)	0.3 to 0.6 m (1 to 2 ft)
38 mm ($1\frac{1}{2}$ in)	0.5 to 0.75 m ($1\frac{1}{2}$ to $2\frac{1}{2}$ ft)
50 mm (2 in)	0.6 to 1.0 m (2 to 3 ft)

Cornell's method

Cornell et al. (1960) reviewed the previously published data and presented empirical equations for predicting the height of the gas and liquid film transfer units. Their correlation takes into account the physical properties of the system, the gas and liquid flow rates, and the column diameter and height. Equations and figures are given for a range of sizes of Raschig rings and Berl saddles. Only those for Berl saddles are given here, as it is unlikely that Raschig rings would be considered for a new column. Though the mass transfer efficiency of Pall rings and INTALOX saddles will be higher than that of the equivalent size Berl saddle, the method can be used to make conservative estimates for these packings.

Bolles and Fair (1982) have extended the correlations given in the earlier paper to include metal Pall rings.

Cornell's equations are:

$$\mathbf{H}_G = 0.011\psi_h (Sc)_v^{0.5} \left(\frac{D_c}{0.305}\right)^{1.11} \left(\frac{Z}{3.05}\right)^{0.33} \Big/ \left(L_w^* f_1 f_2 f_3\right)^{0.5} \tag{17.79}$$

$$\mathbf{H}_L = 0.305\varphi_h (Sc)_L^{0.5} K_3 \left(\frac{Z}{3.05}\right)^{0.15} \tag{17.80}$$

where $\mathbf{H}_G$ = height of a gas-phase transfer unit, m
$\mathbf{H}_L$ = height of a liquid-phase transfer unit, m
$(Sc)_v$ = gas Schmidt number = $(\mu_L/\rho_L D_{LK})$
$(Sc)_L$ = liquid Schmidt number = $(\mu_L/\rho_L D_L)$
D_c = column diameter, m
Z = column height, m
K_3 = percentage flooding correction factor, from Fig. 17.51
ψ_h = $\mathbf{H}_G$ factor from Fig. 17.52
ϕ_h = $\mathbf{H}_L$ factor from Fig. 17.53
L_w^* = liquid mass flow rate per unit area column cross-sectional area, kg/m^{2}s
f_1 = liquid viscosity correction factor = $(\mu_L/\mu_w)^{0.16}$
f_2 = liquid density correction factor = $(\rho_w/\rho_L)^{1.25}$
f_3 = surface tension correction factor = $(\sigma_w/\sigma_L)^{0.8}$

where the suffix w refers to the physical properties of water at 20 °C; all other physical properties are evaluated at the column conditions.

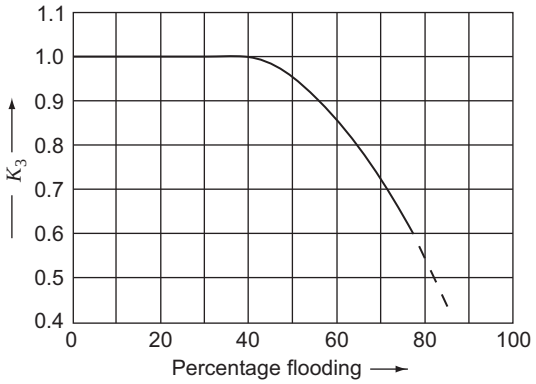


FIG. 17.51 Percentage flooding correction factor.

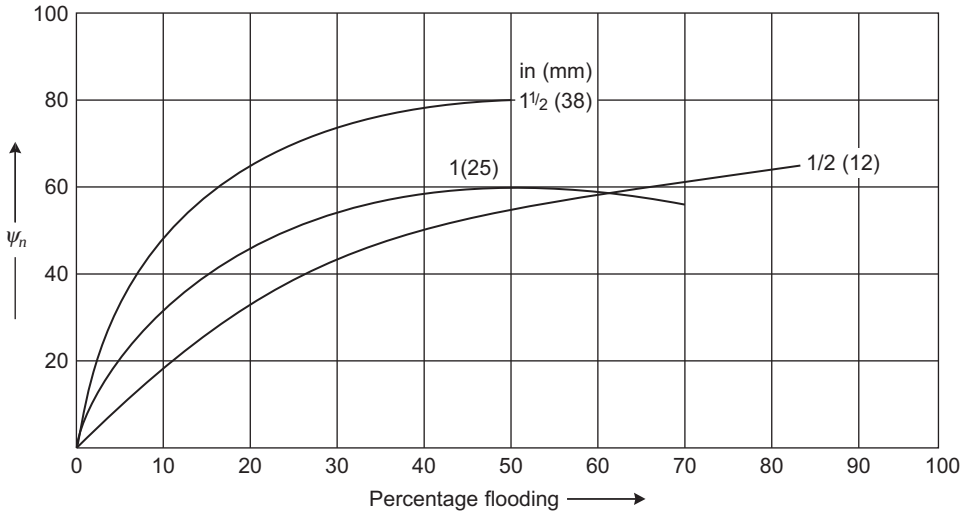


FIG. 17.52 Factor for $\mathbf{H}_G$ for Berl saddles.

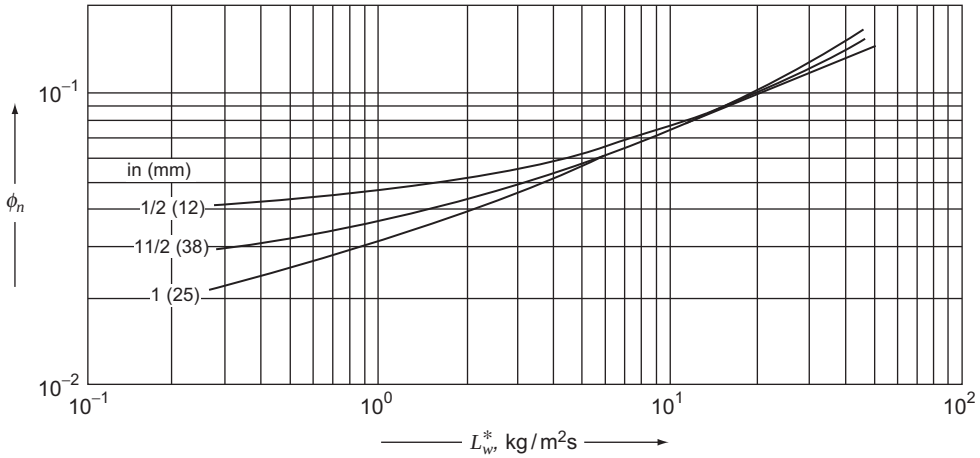


FIG. 17.53 Factor for $\mathbf{H}_L$ for Berl saddles.

The terms $(D_c/0.305)$ and $(Z/3.05)$ are included in the equations to allow for the effects of column diameter and packed-bed height. The "standard" values used by Cornell were 1 ft (0.305 m) for diameter and 10 ft (3.05 m) for height. These correction terms will clearly give silly results if applied over too wide a range of values. For design purposes, the diameter correction term should be taken as a fixed value of 2.3 for columns above 0.6 m (2 ft) diameter, and the height correction should only be included when the distance between liquid redistributors is greater than 3 m. To use Figs. 17.51 and 17.52, an estimate of the column percentage flooding is needed. This can be obtained from Fig. 17.54, where a flooding line has been included with the lines of constant pressure drop.

$$\text{Percentage flooding} = \left[\frac{K_4 \text{ at design pressure drop}}{K_4 \text{ at flooding}}\right]^{1/2} \tag{17.81}$$

Onda's method

Onda et al. (1968) published useful correlations for the film mass transfer coefficients k_G and k_L and the effective wetted area of the packing a_w, which can be used to calculate $\mathbf{H}_G$ and $\mathbf{H}_L$.

Their correlations were based on a large amount of data on gas absorption and distillation, with a variety of packings that included Pall rings and Berl saddles. Their method for estimating the effective area of packing can also be used with experimentally determined values of the mass transfer coefficients and values predicted using other correlations.

The equation for the effective area is:

$$\frac{a_w}{a} = 1 - \exp\left[-1.45\left(\frac{\sigma_c}{\sigma_L}\right)^{0.75}\left(\frac{L_w^*}{a\mu_L}\right)^{0.1}\left(\frac{L_w^{*2}a}{\rho_L^2 g}\right)^{-0.05}\left(\frac{L_w^{*2}}{\rho_L \sigma_L a}\right)^{0.2}\right] \tag{17.82}$$

and for the mass coefficients:

$$k_L\left(\frac{\rho_L}{\mu_L g}\right)^{1/3} = 0.0051\left(\frac{L_w^*}{a_w\mu_L}\right)^{2/3}\left(\frac{\mu_L}{\rho_L D_L}\right)^{-1/2}(ad_p)^{0.4} \tag{17.83}$$

$$\frac{k_G}{a}\frac{RT}{D_v} = K_5\left(\frac{V_w^*}{a\mu_v}\right)^{0.7}\left(\frac{\mu_v}{\rho_v D_v}\right)^{1/3}(ad_p)^{-2.0} \tag{17.84}$$

where $K_5 = 5.23$ for packing sizes above 15 mm and 2.00 for sizes below 15 mm
$L_w^* =$ liquid mass flow rate per unit cross-sectional area, kg/m^{2}s
$V_w^* =$ gas mass flow rate per unit column cross-sectional area, kg/m^{2}s
$a_w =$ effective interfacial area of packing per unit volume, m^2/m^3
$a =$ actual area of packing per unit volume (see Table 17.2), m^2/m^3
$d_p =$ packing size, m

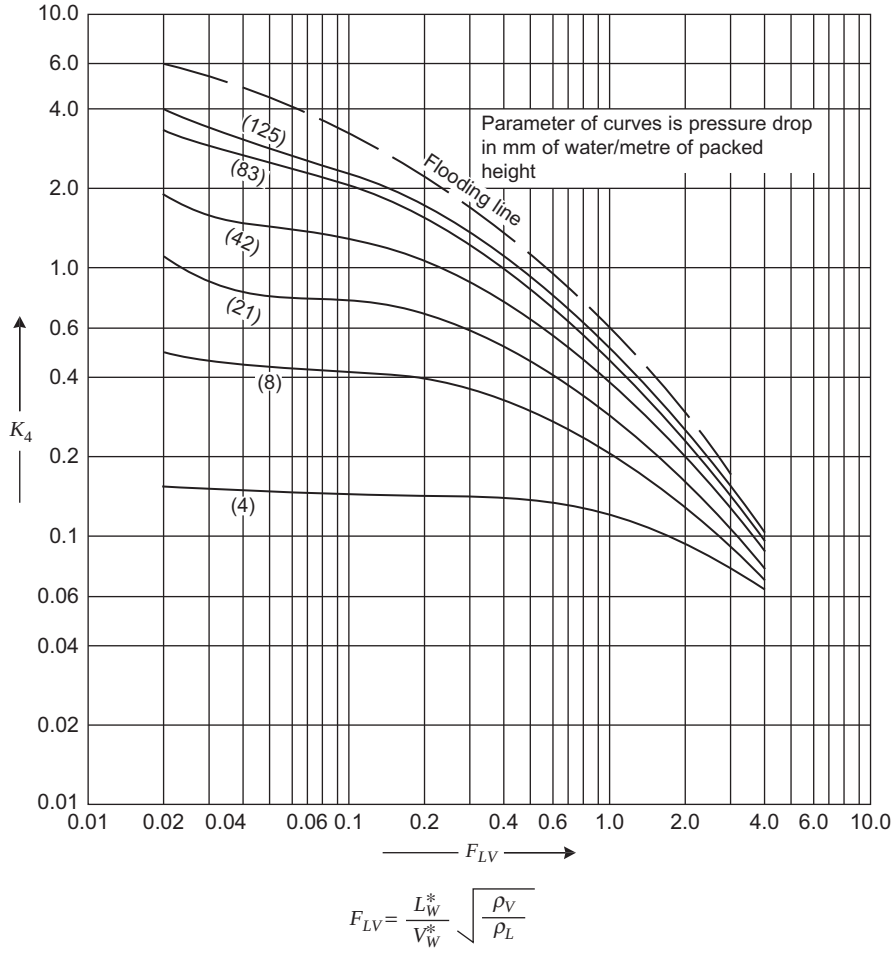


FIG. 17.54 Generalized pressure drop correlation. *(Adapted from a Fig. by Koch-Glitsch, LP, with permission.)*

σ_c = critical surface tension for the particular packing material given here:

Material	σ_c **mN/m**
Ceramic	61
Metal (steel)	75
Plastic (polyethylene)	33
Carbon	56

σ_L = liquid surface tension, N/m

k_G = gas film mass transfer coefficient, kmol/m^{2}s atm or kmol/m^{2}s bar

k_L = liquid film mass transfer coefficient, kmol/m^{2}s (kmol/m^3) = m/s

Note: All the groups in the equations are dimensionless.
The units for k_G will depend on the units used for the gas constant:

$$R = 0.08206 \text{ atm m}^3/\text{kmol K or}$$

$$0.08314 \text{ bar m}^3/\text{kmol K}$$

The film transfer unit heights are given by:

$$\mathbf{H}_G = \frac{G_m}{k_G a_w P} \tag{17.85}$$

$$\mathbf{H}_L = \frac{L_m}{k_L a_w C_t} \tag{17.86}$$

where P = column operating pressure, atm or bar
C_t = total concentration, kmol/m^3 = ρ_L/molecular weight solvent
G_m = molar gas flow rate per unit cross-sectional area, kmol/m^{2}s
L_m = molar liquid flow rate per unit cross-sectional area, kmol/m^{2}s

17.14.4 Column diameter (capacity)

The capacity of a packed column is determined by its cross-sectional area. Normally, the column will be designed to operate at the highest economical pressure drop to ensure good liquid and gas distribution. For random packings, the pressure drop will not normally exceed 80 mm of water per meter of packing height. At this value, the gas velocity will be about 80% of the flooding velocity. Recommended design values, mm water per m packing, are:

Absorbers and strippers	15 to 50
Distillation, atmospheric and moderate pressure	40 to 80

Where the liquid is likely to foam, these values should be halved.

For vacuum distillations, the maximum allowable pressure drop will be determined by the process requirements, but for satisfactory liquid distribution, the pressure drop should not be less than 8 mm water per m. If very low bottom pressures are required, special low-pressure-drop gauze packings should be considered such as Hyperfil, Multifil′ or Dixon rings.

The column cross-sectional area and diameter for the selected pressure drop can be determined from the generalized pressure drop correlation given in Fig. 17.54. Fig. 17.54 correlates the liquid and vapor flow rates, system physical properties and packing characteristics, with the gas mass flow rate per unit cross-sectional area; with lines of constant pressure drop as a parameter.

The term K_4 in Fig. 17.54 is the function:

$$K_4 = \frac{13.1\left(V_w^*\right)^2 F_p \left(\frac{\mu_L}{\rho_L}\right)^{0.1}}{\rho_v(\rho_L - \rho_v)} \tag{17.87}$$

where V_w^* = gas mass flow rate per unit column cross-sectional area, kg/m^{2}s
F_p = packing factor, characteristic of the size and type of packing, see Table 17.2, m^{-1}
μ_L = liquid viscosity, Ns/m^2
ρ_L, ρ_v = liquid and vapor densities, kg/m^3

The values of the flow factor F_{LV} given in Fig. 17.54 cover the range that will generally give satisfactory column performance.

The ratio of liquid to gas flow will be fixed by the reflux ratio in distillation, and in gas absorption will be selected to give the required separation with the most economic use of solvent.

A new generalized correlation for pressure drop in packed columns, similar to Fig. 17.54, has been published by Leva (1992, 1995). The new correlation gives a better prediction for systems where the density of the irrigating fluid is appreciably greater than that of water. It can also be used to predict the pressure drop over dry packing.

Example 17.9

Sulfur dioxide produced by the combustion of sulfur in air is absorbed in water. Pure SO_2 is then recovered from the solution by steam stripping. Make a preliminary design for the absorption column. The feed will be 5000 kg/h of gas containing 8% v/v SO_2. The gas will be cooled to 20 °C. A 95% recovery of the sulfur dioxide is required.

Solution

As the solubility of SO_2 in water is high, operation at atmospheric pressure should be satisfactory. The feed-water temperature will be taken as 20 °C, a reasonable design value.

Solubility data

From Green and Southard (2018):

SO2	% w/w solution	0.05	0.1	0.15	0.2	0.3	0.5	0.7	1.0	1.5
	Partial press. gas mmHg	1.2	3.2	5.8	8.5	14.1	26	39	59	92

These data are plotted in Fig. 17.55.

Number of stages

Partial pressure in the exit gas at 95% recovery $= 60.8 \times 0.05 = 3.04$ mmHg

Over this range of partial pressure, the equilibrium line is essentially straight, so Fig. 17.49 can be used to estimate the number of stages needed.

The use of Fig. 17.49 will slightly overestimate the number of stages, and a more accurate estimate would be made by graphical integration of Equation 17.72, but this is not justified in view of the uncertainty in the prediction of the transfer unit height.

$$\text{Molecular weights: } SO_2 = 64,\ H_2O = 18, \text{air} = 29$$

Slope of equilibrium line

From the data: partial pressure at 1.0% w/w $SO_2 = 59$ mmHg.

$$\text{Mole fraction in vapor} = \frac{59}{760} = 0.0776$$

$$\text{Mole fraction in liquid} = \frac{\frac{1}{64}}{\frac{1}{64} + \frac{99}{18}} = 0.0028$$

$$m = \frac{0.0776}{0.0028} = 27.4$$

To decide the most economic water flow rate, the stripper design should be considered together with the absorption design, but for the purpose of this example, the absorption design will be considered alone. Using Fig. 17.49, the number of stages required at different water rates will be determined and the "optimum" rate chosen:

$$\frac{y_1}{y_2} = \frac{p_1}{p_2} = \frac{60.8}{3.04} = 20$$

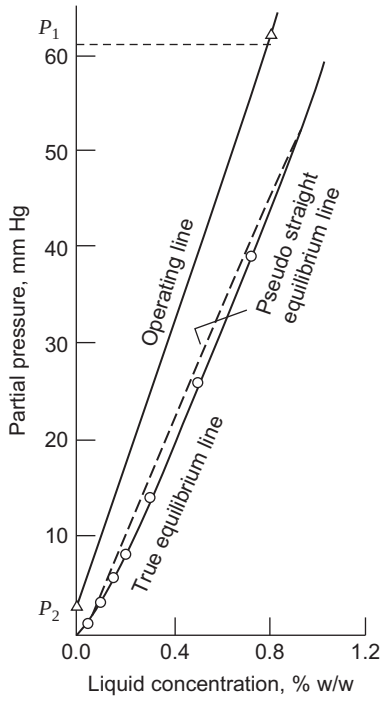


FIG. 17.55 SO_2 absorber design (Example 17.9).

$m\frac{G_m}{L_m}$	0.5	0.6	0.7	0.8	0.9	1.0
N_{OG}	3.7	4.1	6.3	8	10.8	19.0

It can be seen that the "optimum" will be between $mG_m/L_m = 0.6$ and 0.8, as would be expected. Below 0.6 there is only a small decrease in the number of stages required with increasing liquid rate; above 0.8 the number of stages increases rapidly with decreasing liquid rate.

Check the liquid outlet composition at 0.6 and 0.8:

$$\text{Material balance } L_m x_1 = G_m(y_1 - y_2)$$

$$\text{so} x_1 = \frac{G_m}{L_m}(0.08 \times 0.95) = \frac{m}{27.4}\frac{G_m}{L_m}(0.076)$$

$$\text{at} \frac{mG_m}{L_m} = 0.6, x_1 = 1.66 \times 10^{-3} \text{ mol fraction}$$

$$\text{at} \frac{mG_m}{L_m} = 0.8, x_1 = 2.22 \times 10^{-3} \text{ mol fraction}$$

Use 0.8, as the higher concentration will favor the stripper design and operation without significantly increasing the number of stages needed in the absorber.

$$N_{OG} = \underline{\underline{8}}$$

Column diameter

The physical properties of the gas can be taken as those for air, as the concentration of SO_2 is low.

$$\text{Gas flow} - \text{rate} = \frac{5000}{3600} = 1.39 \text{ kg/s}, \ = \frac{1.39}{29} = 0.048 \text{ kmol/s}$$

$$\text{Liquid flow} - \text{rate} = \frac{27.4}{0.8} \times 0.048 = 1.64 \text{ kmol/s}$$

$$= 29.5 \text{ kg/s}.$$

Select 38 mm ($1\frac{1}{2}$ in) ceramic INTALOX saddles.

From Table 17.2, $F_p = 170 \text{ m}^{-1}$:

$$\text{Gas density at } 20^\circ\text{C} = \frac{29}{22.4} \times \frac{273}{293} = 1.21 \text{ kg/m}^3$$

$$\text{Liquid density} \approx 1000 \text{ kg/m}^3$$

$$\text{Liquid viscosity} = 10^{-3} \text{Ns/m}^2$$

$$\frac{L_W^*}{V_W^*}\sqrt{\frac{\rho_v}{\rho_L}} = \frac{29.5}{1.39}\sqrt{\frac{1.21}{10^3}} = 0.74$$

Design for a pressure drop of 20 mm H_2O/m packing:

From Fig. 17.54,

$$K_4 = 0.35$$

$$\text{At flooding } K_4 = 0.8$$

$$\text{Percentage flooding} = \sqrt{\frac{0.35}{0.8}} \times 100 = 66\ \%, \text{ satisfactory.}$$

From Equation 17.87:

$$V_W^* = \left[\frac{K_4\rho_V(\rho_L-\rho_v)}{13.1F_p(\mu_L/\rho_L)^{0.1}}\right]^{1/2}$$

$$= \left[\frac{0.35\times 1.21(1000-1.21)}{13.1\times 170(10^{-3}/10^3)^{0.1}}\right]^{1/2} = 0.87 \text{ kg/m}^2\text{s}$$

$$\text{Column area required} = \frac{1.39}{0.87} = 1.6 \text{ m}^2$$

$$\text{Diameter} = \sqrt{\frac{4}{\pi}\times 1.6} = 1.43 \text{ m}$$

Round off to <u>1.50 m</u>

$$\text{Column area} = \frac{\pi}{4}\times 1.5^2 = 1.77 \text{ m}^2$$

$$\text{Packing size to column diameter ratio} = \frac{1.5}{38\times 10^{-3}} = 39$$

A larger packing size could be considered.
Percentage flooding at selected diameter:

$$= 66\times\frac{1.6}{1.77} = 60\ \%$$

Could consider reducing column diameter to the nearest standard pipe size.

Estimation of H_{OG}

Cornell's method

$$D_L = 1.7\times 10^{-9}\text{m}^2/\text{s}$$

$$D_v = 1.45\times 10^{-5}\text{m}^2/\text{s}$$

$$\mu_v = 0.018\times 10^{-3}\text{Ns/m}^2$$

$$(Sc)_v = \frac{0.018\times 10^{-3}}{1.21\times 1.45\times 10^{-5}} = 1.04$$

$$(Sc)_L = \frac{10^{-3}}{1000\times 1.7\times 10^{-9}} = 588$$

$$L_W^* = \frac{29.5}{1.77} = 16.7 \text{ kg/s m}^2$$

From Fig. 17.51, at 60% flooding, $K_3 = 0.85$.
From Fig. 17.52, at 60% flooding, $\psi_h = 80$.
From Fig. 17.53, at $L_W^* = 16.7$, $\phi_h = 0.1$.

$\mathbf{H}_{OG}$ can be expected to be around 1 m, so as a first estimate Z can be taken as 8 m. The column diameter is greater than 0.6 m, so the diameter correction term will be taken as 2.3.

$$\mathbf{H}_L = 0.305\times 0.1(588)^{0.5}\times 0.85\left(\frac{8}{3.05}\right)^{0.15} = 0.7 \text{ m} \tag{17.80}$$

As the liquid temperature has been taken as 20 °C and the liquid is water:

$$f_1 = f_2 = f_3 = 1$$

$$\mathbf{H}_G = 0.011 \times 80(1.04)^{0.5}(2.3)\left(\frac{8}{3.05}\right)^{0.33} \Big/ (16.7)^{0.5} = 0.7 \text{ m} \tag{17.79}$$

$$\mathbf{H}_{OG} = 0.7 + 0.8 \times 0.7 = 1.3 \text{ m}$$
$$Z = 8 \times 1.3 = 10.4 \text{ m, close enough to the estimated value.} \tag{17.73}$$

Onda's method

$R = 0.08314$ bar m^3/kmol.K.

Surface tension of liquid, taken as water at 20°C $= 70 \times 10^{-3}$N/m

$g = 9.81$ m/s^2

$d_p = 38 \times 10^{-3}$m

From Table 17.3, for 38 mm INTALOX saddles:

$$a = 194 \text{ m}^2/\text{m}^3$$

σ_c for ceramics $= 61 \times 10^{-3}$ N/m

$$\frac{a_W}{a} = 1 - \exp\left[-1.45\left(\frac{61 \times 10^{-3}}{70 \times 10^{-3}}\right)^{0.75}\left(\frac{17.6}{194 \times 10^{-3}}\right)^{0.1}\left(\frac{17.6^2 \times 194}{1000^2 \times 9.81}\right)^{-0.05} \times \left(\frac{17.6^2}{1000 \times 70 \times 10^{-3} \times 194}\right)^{0.2}\right] = 0.71 \tag{17.82}$$

$$a_W = 0.71 \times 194 = 138 \text{ m}^2/\text{m}^3$$

$$k_L\left(\frac{10^3}{10^{-3} \times 9.81}\right)^{1/3} = 0.0051\left(\frac{17.6}{138 \times 10^{-3}}\right)^{2/3}\left(\frac{10^{-3}}{10^3 \times 1.7 \times 10^{-9}}\right)^{-1/2} \times \left(194 \times 38 \times 10^{-3}\right)^{0.4}$$

$$k_L = 2.5 \times 10^{-4} \text{ m/s} \tag{17.83}$$

$$V_W^* \text{ on actual column diameter } \frac{1.39}{1.77} = 0.79 \text{ kg/m}^2\text{s}$$

$$k_G \frac{0.08314 \times 293}{194 \times 1.45 \times 10^{-5}} = 5.23\left(\frac{0.79}{194 \times 0.018 \times 10^{-3}}\right)^{0.7} \times \left(\frac{0.018 \times 10^{-3}}{1.21 \times 1.45 \times 10^{-5}}\right)^{1/3}\left(194 \times 38 \times 10^{-3}\right)^{-2.0}$$

$$k_G = 5.0 \times 10^{-4} \text{kmol/sm}^2 \text{ bar}$$

$$G_m = \frac{0.79}{29} = 0.027 \text{ kmol/m}^2\text{s} \tag{17.84}$$

$$L_m = \frac{16.7}{18} = 0.93 \text{ kmol/m}^2\text{s}$$

$$\mathbf{H}_G = \frac{0.027}{5.0 \times 10^{-4} \times 138 \times 1.013} = 0.39 \text{ m}$$

$$C_T = \text{total concentration, as water,} \tag{17.85}$$

$$= \frac{1000}{18} = 55.5 \text{ kmol/m}^3$$

$$\mathbf{H}_L = \frac{0.93}{2.5 \times 10^{-4} \times 138 \times 55.6} = 0.49 \text{ m} \tag{17.86}$$

$$\mathbf{H}_{OG} = 0.39 + 0.8 \times 0.49 = \underline{\underline{0.78 \text{ m}}} \tag{17.73}$$

Use higher value, estimated using Cornell's method, and round up packed-bed height to $\underline{\underline{11 \text{ m}}}$.

17.14.5 Column internals

The internal fittings in a packed column are simpler than those in a plate column but must be carefully designed to ensure good performance. As a general rule, the standard fittings developed by the packing manufacturers should be specified. Some typical designs are shown in Figs. 17.56 to 17.65, and their use is discussed in the following paragraphs.

Packing support

The function of the support plate is to carry the weight of the wet packing while allowing free passage of the gas and liquid. These requirements conflict; a poorly designed support will give a high pressure drop and can cause local flooding. Simple grid and perforated plate supports are used, but in these designs the liquid and gas have to vie for the same openings. Wide-spaced grids are used to increase the flow area, with layers of larger-size packing stacked on the grid to support the small-size random packing (Fig. 17.56).

The best design of packing support is one in which gas inlets are provided above the level where the liquid flows from the bed, such as the gas-injection type shown in Figs. 17.57 and 17.58. These designs have a low pressure drop and no tendency to flooding. They are available in a wide range of sizes and materials: metals, ceramics, and plastics.

Liquid distributors

The satisfactory performance of a plate column is dependent on maintaining a uniform flow of liquid throughout the column, and good initial liquid distribution is essential. Various designs of distributors are used. For small-diameter columns a central open feed pipe, or one fitted with a spray nozzle, may well be adequate, but for larger columns more elaborate designs are needed to ensure good distribution at all liquid flow rates. The two most commonly used designs are the orifice type, shown in Fig. 17.59, and the weir type, shown in Fig. 17.60. In the orifice

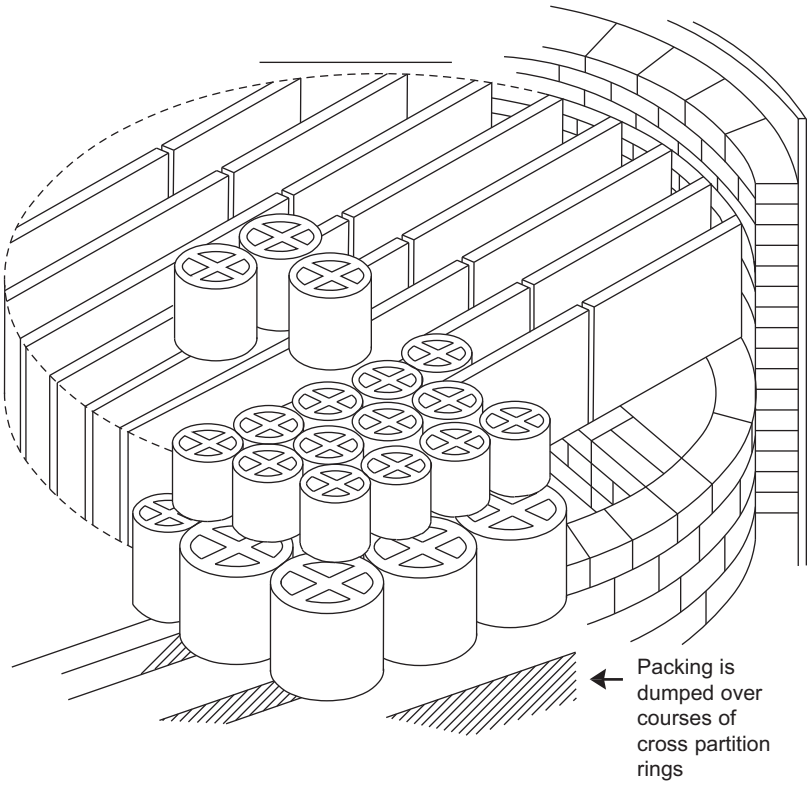


FIG. 17.56 Stacked packing used to support random packing.

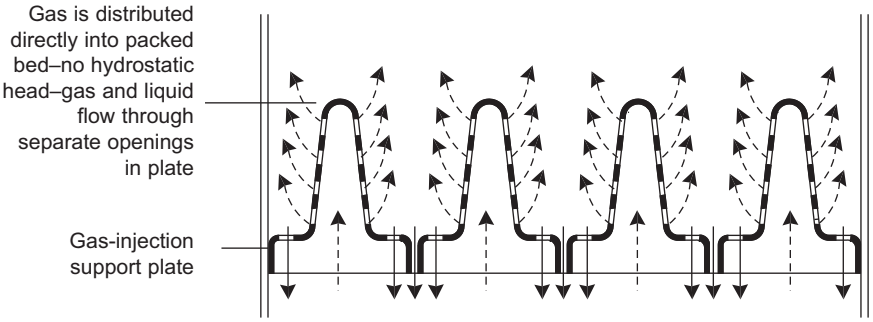


FIG. 17.57 The principle of the gas-injection packing support.

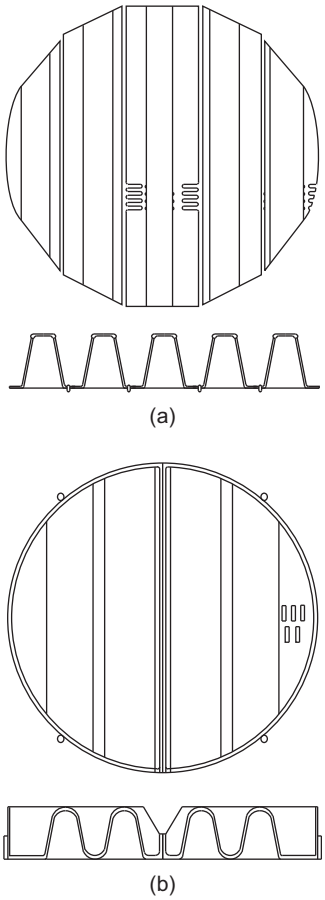


FIG. 17.58 Typical designs of gas-injection supports (Koch-Glitsch, LP). (a) Small-diameter columns. (b) Large-diameter columns.

type the liquid flows through holes in the plate and the gas through short stand pipes. The gas pipes should be sized to give sufficient area for gas flow without creating a significant pressure drop; the holes should be small enough to ensure that there is a level of liquid on the plate at the lowest liquid rate but large enough to prevent the distributor overflowing at the highest rate. In the weir type the liquid flows over notched weirs in the gas stand pipes. This type can be designed to cope with a wider range of liquid flow rates than the simpler orifice type.

For large-diameter columns, the trough-type distributor shown in Fig. 17.61 can be used and will give good liquid distribution with a large free area for gas flow.

All distributors that rely on the gravity flow of liquid must be installed in the column level, or maldistribution of liquid will occur.

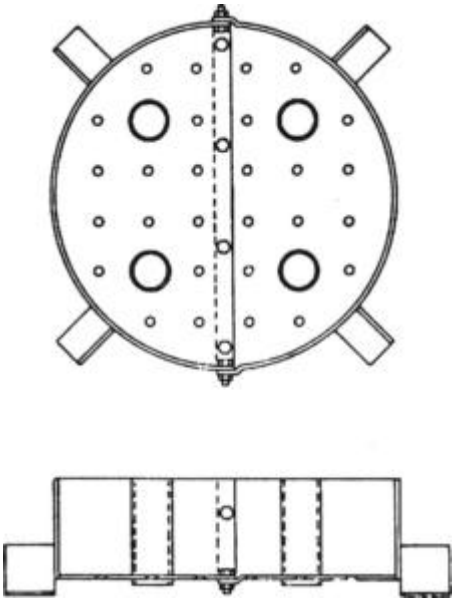


FIG. 17.59 Orifice-type distributor (Koch-Glitsch, LP).

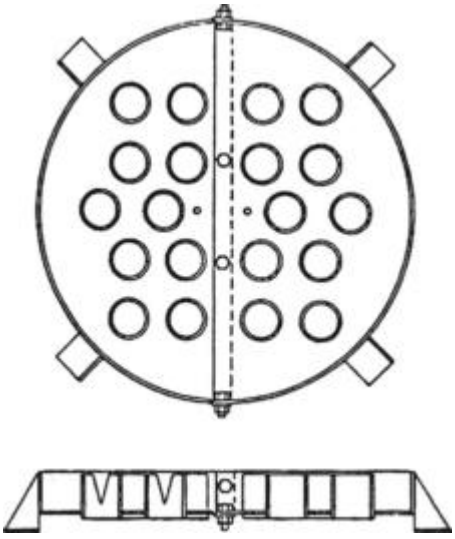


FIG. 17.60 Weir-type distributor (Koch-Glitsch, LP).

A pipe manifold distributor (Fig. 17.62) can be used when the liquid is fed to the column under pressure and the flow rate is reasonably constant. The distribution pipes and orifices should be sized to give an even flow from each element.

Liquid redistributors

Redistributors are used to collect liquid that has migrated to the column walls and redistribute it evenly over the packing. They will also even out any maldistribution that has occurred within the packing.

A full redistributor combines the functions of a packing support and a liquid distributor; a typical design is shown in Fig. 17.63.

The "wall-wiper" type of redistributor, in which a ring collects liquid from the column wall and redirects it into the center packing, is occasionally used in small-diameter columns, less than 0.6 m. Care should be taken when specifying this type to select a design that does not unduly restrict the gas flow and cause local flooding. A good design is that shown in Fig. 17.64.

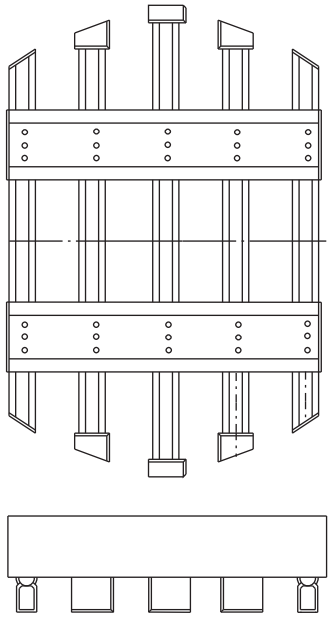


FIG. 17.61 Weir-trough distributors (Koch-Glitsch, LP).

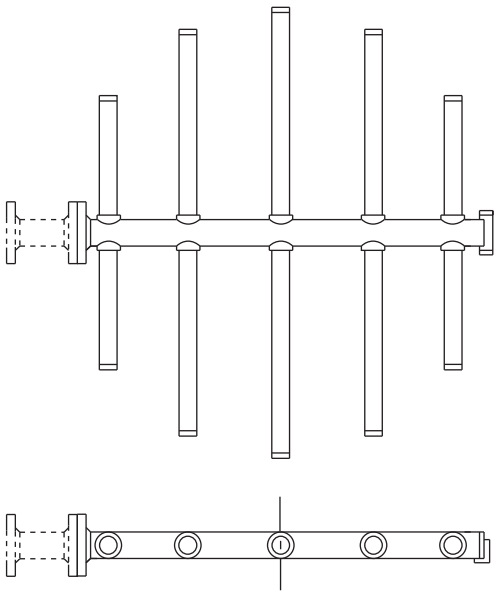


FIG. 17.62 Pipe distributor (Koch-Glitsch, LP).

The maximum bed height that should be used without liquid redistribution depends on the type of packing and the process. Distillation is less susceptible to maldistribution than absorption and stripping. As a general guide, the maximum bed height should not exceed 3 column diameters for Raschig rings and 8 to 10 for Pall rings and saddles. In a large-diameter column the bed height will also be limited by the maximum weight of packing that can be supported by the packing support and column walls; this will be around 8 m.

Hold-down plates

At high gas rates, or if surging occurs through misoperation, the top layers of packing can be fluidized. Under these conditions ceramic packing can break up and the pieces filter down the column and plug the packing; metal and plastic packing can be blown out of the column. Hold-down plates are used with ceramic packing to weigh down the top layers and prevent fluidization; a typical design is shown in Fig. 17.65. Bed limiters are sometimes used with plastic and metal

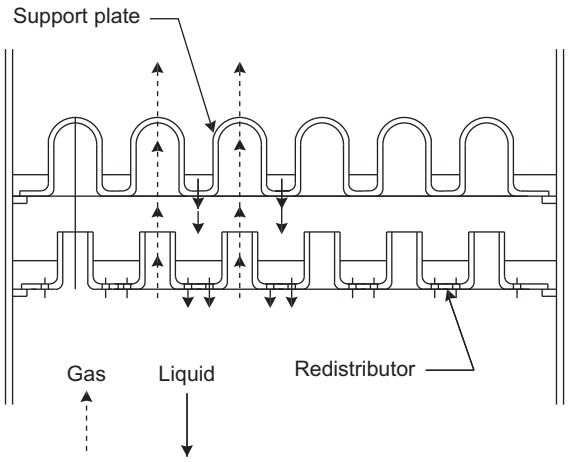


FIG. 17.63 Full redistributor.

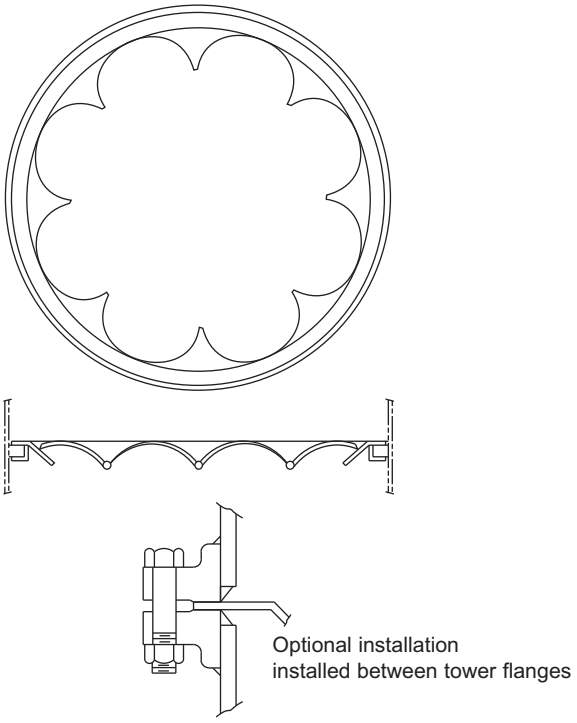


FIG. 17.64 "Wall-wiper" redistributor (Koch-Glitsch, LP).

packings to prevent expansion of the bed when operating at a high pressure drop. They are similar to hold-down plates but are of lighter construction and are fixed to the column walls. The openings in hold-down plates and bed limiters should be small enough to retain the packing, but should not restrict the gas and liquid flow.

Installing packing

Ceramic and metal packings are normally dumped into the column "wet" to ensure a truly random distribution and prevent damage to the packing. The column is partially filled with water and the packing dumped into the water. A height of water must be kept above the packing at all times.

If the columns must be packed dry, for instance, to avoid contamination of process fluids with water, the packing can be lowered into the column in buckets or other containers. Ceramic packings should not be dropped from a height of more than half a meter.

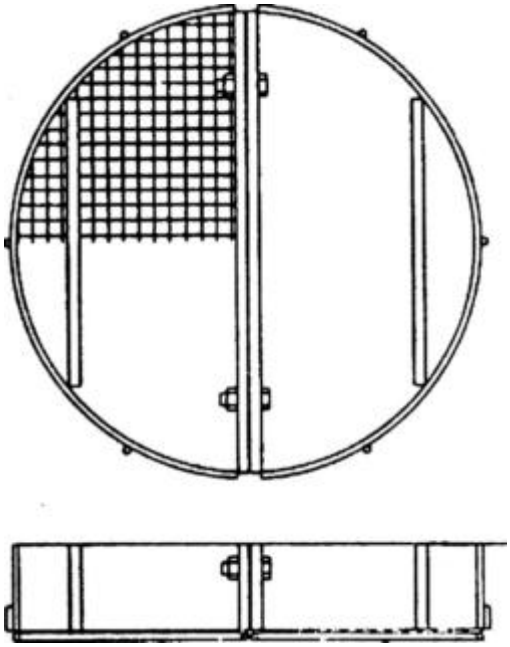


FIG. 17.65 Hold-down plate design (Koch-Glitsch, LP).

Liquid hold-up

An estimate of the amount of liquid held up in the packing under operating conditions is needed to calculate the total load carried by the packing support. The liquid hold-up depends on the liquid rate and, to some extent, on the gas flow rate. The packing manufacturer's design literature should be consulted to obtain accurate estimates. As a rough guide, a value of about 25% of the packing weight can be taken for ceramic packings.

17.14.6 Wetting rates

If very low liquid rates must be used, outside the range of F_{LV} given in Fig. 17.54, the packing wetting rate should be checked to make sure it is above the minimum recommended by the packing manufacturer.

Wetting rate is defined as:

$$\text{wetting rate} = \frac{\text{volumetric liquid rate per unit cross} - \text{sectional area}}{\text{packing surface area per unit volume}}$$

A nomograph for the calculation of wetting rates is given in Chhabra and Gurappa (2019).

Wetting rates are frequently expressed in terms of mass or volume flow rate per unit column cross-sectional area. Kister (1992) gives values for minimum wetting rates of 0.5 to 2 gpm/ft^2 (0.35×10^{-3} to 1.4×10^{-3} m^3 s^{-1}/m^2) for random packing and 0.1 to 0.2 gpm/ft^2 (0.07×10^{-3} to 0.14×10^{-3} m^3 s^{-1}/m^2) for structured packing. Norman (1961) recommends that the liquid rate in absorbers should be kept above 2.7 kg/m^{2}s.

If the design liquid rate is too low, the diameter of the column should be reduced. For some processes liquid can be recycled to increase the flow over the packing.

A substantial factor of safety should be applied to the calculated bed height for processes where the wetting rate is likely to be low, and less space should be allowed between liquid redistributors.

17.15 Column auxiliaries

Intermediate storage tanks are sometimes used to smooth out fluctuations in column operation and process upsets, for example, when a batch reactor section feeds a continuous distillation section. These tanks should be sized

to give sufficient hold-up time for smooth operation and control. The hold-up time required will depend on the nature of the process and on how critical the operation is; some typical values for distillation processes are given here:

Operation	Time, minutes
Feed to a train of columns	10–20
Between columns	5–10
Feed to a column from storage	2–5
Reflux drum	5–15

The time given is that for the level in the tank to fall from the normal operating level to the minimum operating level if the feed ceases.

Horizontal or vertical tanks are used, depending on the size and duty. Where only a small hold-up volume is required, this can be provided by adding volume to the sump of the upstream column by extending the column base or, for reflux accumulators, by extending the bottom header of the condenser.

The specification and sizing of surge tanks and accumulators are discussed in more detail by Mehra (1979) and Evans (1980).

The design of condensers is discussed in Section 19.10, and the design of reboilers is covered in Section 19.11. The control of distillation columns is addressed in Section 5.4.7.

17.16 Solvent extraction (liquid–liquid extraction)

Extraction should be considered as an alternative to distillation in the following situations:

1. When the components in the feed have close boiling points. Extraction in a suitable solvent may be more economic if the relative volatility is below 1.2.
2. If the feed components form an azeotrope.
3. If the solute is heat sensitive and can be extracted into a lower-boiling solvent to reduce the thermal history during recovery.

Solvent selection

The following factors must be considered when selecting a suitable solvent for a given extraction:

1. Phase equilibrium: The distribution coefficient or partition coefficient, K, is the ratio of the mole fractions in each phase: $x_\alpha = K\, x_\beta$. The distribution coefficient is analogous to the equilibrium constant in absorption. The relative separation or selectivity is a measure of the distribution of two solutes between the two solvents and is the ratio of the distribution coefficients for the two solutes. Selectivity is analogous to relative volatility in distillation. The greater the difference in solubility of the preferred solute between the two solvents, the easier it will be to extract. This is particularly important when trying to preferentially extract one component from a mixture, as often occurs in the recovery of fermentation products and specialty chemicals.
2. Partition ratio: This is the weight fraction of the solute in the extract divided by the weight fraction in the raffinate. This determines the quantity of solvent and number of stages needed. The less solvent needed, the lower the solvent and solvent recovery costs.
3. Density: The greater the density difference between the feed and extraction solvents, the easier it will be to separate the solvents.
4. Miscibility: Ideally, the two solvents should be immiscible. The greater the solubility of the extraction solvent in the feed solvent, the more difficult it will be to recover the solvent from the raffinate and the higher the cost.
5. Safety: Whenever it is possible and economical, a solvent should be chosen that is not toxic or dangerously flammable.
6. Cost: The purchase cost of the solvent is important but should not be considered in isolation from the total process costs. It may be worth considering a more expensive solvent if it is more effective and easier to recover.

17.16.1 Extraction equipment

Extraction equipment can be divided into two broad groups:

1. Stage-wise extractors, in which the liquids are alternately contacted (mixed) and then separated in a series of stages. The "mixer–settler" contactor is an example of this type. Several mixer–settlers are often used in series to increase the effectiveness of the extraction.

2. Differential extractors, in which the phases are continuously in contact in the extractor and are only separated at the exits, for example, in packed-column extractors.

Extraction columns can be further subdivided according to the method used to promote contact between the phases: packed, plate, mechanically agitated, or pulsed columns. Various types of proprietary centrifugal extractors are also used.

The following factors should be taken into consideration when selecting an extractor for a particular application:

1. The number of stages required
2. The throughputs
3. The settling characteristics of the phases
4. The available floor area and headroom

Hanson (1968) has given a selection guide based on these factors, which can be used to select the type of equipment most likely to be suitable (Fig. 17.66). Additional guidance is given in the paper by Koch and Shiveler (2015).

The basic principles of liquid–liquid extraction are covered in several specialist texts: Treybal (1980), Robbins (1997), and Humphrey and Keller (1997).

17.16.2 Extractor design

Number of stages

The primary task in the design of an extractor for a liquid–liquid extraction process is the determination of the number of stages needed to achieve the separation required.

The stages may be arranged in three ways:

1. Fresh solvent fed to each stage, the raffinate passing from stage to stage (cross-flow)
2. The extracting solvent fed co-currently with the raffinate, from stage to stage (co-current flow)
3. The exacting solvent fed countercurrent to the raffinate (countercurrent flow)

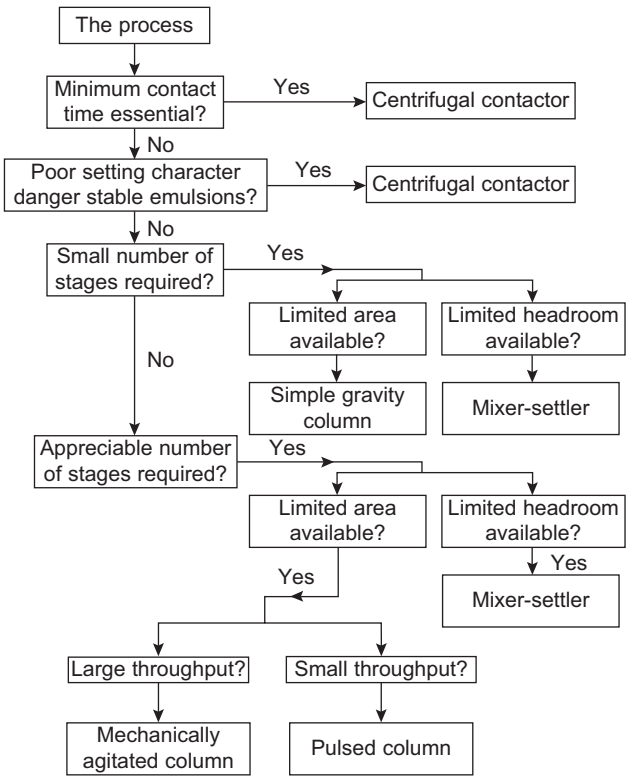


FIG. 17.66 Selection guide for liquid–liquid contactors. *From Hanson, 1968.*

Countercurrent flow is the most efficient method and the most commonly used. It will give the greatest concentration of the solute in the extract and the least use of solvent.

Equilibrium data

To determine the number of stages, it is best to plot the equilibrium data on a triangular diagram (Fig. 17.67). Each corner of the triangle represents 100% of the feed solvent, solute or extraction solvent. Each side represents the composition of one of the binary pairs. The ternary compositions are shown in the interior of the triangle. Mixtures within the region bounded by the curve will separate into two phases. The tie lines link the equilibrium compositions of the separate phases. The tie lines reduce in length toward the top of the curve. The point where they disappear is called the *plait* point.

A fuller discussion of the various classes of diagrams used to represent liquid−liquid equilibria is given in Chhabra and Gurappa (2019); see also Treybal (1980) and Humphrey et al. (1984).

The most comprehensive source of equilibrium data for liquid−liquid systems is the DECHEMA data series (Sorensen & Arlt, 1979). Equilibrium data for some systems are also given by Green and Southard (2018). Most commercial process simulation programs can be used to make initial estimates of liquid−liquid equilibria using a three-phase flash operation. Care is needed in selecting an appropriate phase equilibrium model. The UNIQUAC and UNIFAC equations can be used to estimate liquid−liquid equilibria; see Chapter 4. The size of the two-phase region can be highly sensitive to temperature, and it is usually a good idea to use a process simulation program to generate sufficient data to plot the triangular diagram at several temperatures. Care must be taken to ensure that the simulation model is tuned to accurately predict any available experimental data.

Number of stages

The number of stages required for a given separation can be determined from the triangular diagram using a method analogous to the McCabe−Thiele method for distillation. The method set out here is for countercurrent extraction.

Procedure

Refer to Figs. 17.67 and 17.68.

Let the flow rates be:

F = feed of the solution to be extracted
E = extract
R = raffinate
S = the extracting solvent

and the compositions:

r = raffinate
e = extract
s = solvent
f = feed

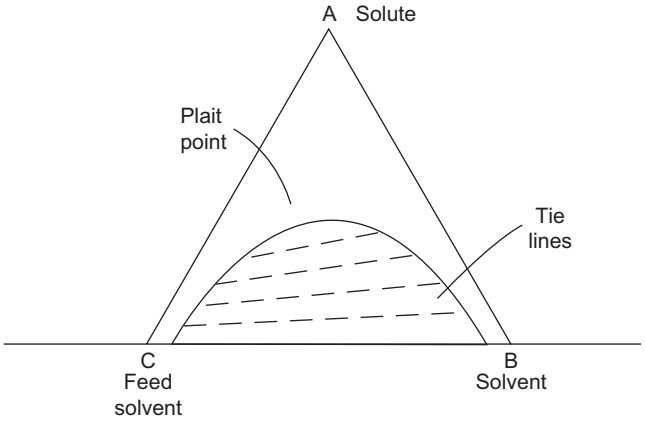


FIG. 17.67 Equilibrium diagram solute distributed between two solvents.

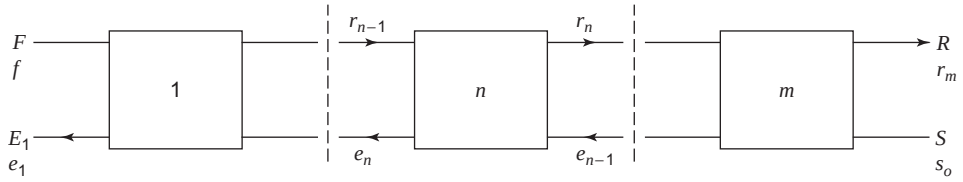


FIG. 17.68 Countercurrent extraction.

Then a material balance over stage n gives:

$$F + E_{n+1} = R_n + E_1$$

It can be shown that the difference in flow rate between the raffinate leaving any stage, R_n, and the extract entering the stage, E_n, is constant. It can also be shown that the difference between the amounts of each component entering and leaving a stage is constant. This means that if lines are drawn on the triangular diagram linking the composition of the raffinate from a stage and the extract entering from the next stage, they will pass through a common pole when extrapolated. The number of stages needed can be found by making use of this construction and the equilibrium compositions given by the tie lines.

Construction

1. Draw the liquid–liquid equilibrium data on triangular graph paper. Show sufficient tie lines to enable the equilibrium compositions to be determined at each stage.
2. Mark the feed and extraction-solvent compositions on the diagram. Join them with a line. The composition of a mixture of the feed and solvent will lie on this line.
3. Calculate the composition of the mixture given by mixing the feed with the extraction solvent. Mark this point, O, on the line drawn in step 2.
4. Mark the final raffinate composition, r_m, on the equilibrium curve.
5. Draw a line from r_m through point O. This will cut the curve at the final extract composition, e_1.
   Note: If the extract composition is specified rather than the raffinate, draw the line from e_1 through O to find r_m.
6. Draw a line from the solvent composition, S_0, through r_m and extend it beyond r_m.
7. Draw a line from e_1 through f and extend it to cross the line drawn in step 6 at the pole point, P.
8. Find the composition of the raffinate leaving the first stage, r_1, by judging the position of the tie line from e_1. Draw a line from the pole point, P, through r_1 to cut the curve at e_2, the extract leaving stage 2.
9. Repeat this procedure until sufficient stages have been drawn to reach the desired raffinate final composition.

If an extended tie line passes through the pole point, P, an infinite number of stages will be needed. This condition sets the minimum flow of extraction-solvent required. It is analogous to a pinch point in distillation.

The method is illustrated in Example 17.10.

Example 17.10

Acetone is to be extracted from a solution in water using 1,1,2-trichloroethane. The feed concentration is 45.0% w/w acetone. Determine the number of stages required to reduce the concentration of acetone to below 10% using 32 kg of extraction solvent per 100 kg feed.

The equilibrium data for this system are given by Treybal et al. (1946).

Solution

Composition of feed + solvent, point O = 0.45 × 100/(100 + 32) = 0.34 = 34%.

Draw line from TCE (trichloroethane) = 100%, point s_0, to feed composition, f, 45% acetone.

Mark point O on this line at 34% acetone.

Mark required final raffinate composition, r_m, on the equilibrium curve at 10%.

Draw line from this point through point O to find final extract composition, e_1.

Draw line from this point though the feed composition, f, and extend this line to cut a line extended from s_0 through r_m, at P.

Using the tie lines plotted on the figure, judge the position that a tie line would have from e_1 and mark it in to find the point on the curve giving the composition of the raffinate leaving the first stage, r_1.
Draw a line through from the pole point, P, through r_1, to find the point on the curve giving the extract composition leaving the second stage, e_2.
Repeat these steps until the raffinate composition found is below 10%.
From Fig. 17.69, it can be seen that five stages are needed.

In this example, the fact that the raffinate composition from stage 5 passes through the specified raffinate composition of 10% is fortuitous. As the construction, particularly the judgment of the position of the tie lines, is approximate, the number of stages should be increased to six. This should ensure that the specified raffinate composition of below 10% is met.

Immiscible solvents

If the solvents are immiscible, the procedure for determining the number of stages required is simplified. The equilibrium curve can be drawn on regular, orthogonal graph paper. An operating line giving the relationship between the compositions of the raffinate and extracts entering and leaving each stage can then be drawn and the stages stepped off. The procedure is similar to the McCabe–Thiele construction for determining the number of stages in distillation; see Section 17.5.2. The slope of the operating line is the ratio of the final raffinate to fresh solvent flow rates. Alternatively, the methods given in Section 17.14.2 for design of absorption columns can be used, where G is the flow rate of the initial solvent phase, L is the flow rate of the extraction solvent, y is the mole fraction of solute in the initial solvent, and m is the partition coefficient.

For a full discussion of the methods that can be used to determine the stage requirements in liquid–liquid extraction, refer to Treybal (1980), Green and Southard (2018), and Robbins (1997). Computer programs are available for the design of extraction processes and are included in the various commercial process simulation packages available; see Chapter 4. It is usually a good practice to make a few hand calculations to determine a good initialization for the process simulation model. At a minimum, the designer should estimate the partition coefficient and ensure that the absorption factor $mG/L \leq 1$ if the goal is to obtain a high recovery of solute.

17.16.3 Extraction columns

The simplest form of extractor is a spray column. The column is empty; one liquid forms a continuous phase and the other liquid flows up or down the column in the form of droplets. Mass transfer takes place to or from the droplets to the continuous phase. The efficiency of a spray tower will be low, particularly with large-diameter columns, due to back-mixing. The efficiency of the basic, empty spray column can be improved by installing plates or packing.

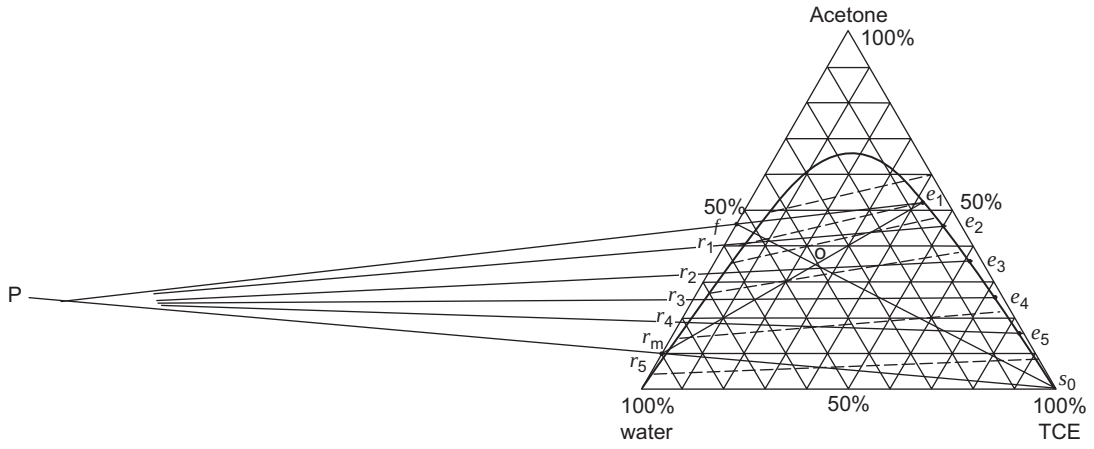


FIG. 17.69 Example 17.10.

Sieve plates are used, similar to those used for distillation and absorption. The plates can be designed so that either the heavy phase is dispersed in the light phase (sometimes called "rain decks") or the light phase is dispersed in the heavy phase ("reverse rain decks").

Random packings are also used; they are the same as those used in packed distillation and absorption columns. The properties of random packings are given in Tables 17.2 and 17.3. Proprietary structured packings are also used. Criteria for selection of column internals are given by Koch and Shiveler (2015).

Mass transfer in packed columns is a continuous, differential process, so the transfer unit method should be used to determine the column height, as used in absorption; see Section 17.14.2. It is often convenient to treat packed extraction columns as staged processes and use the HETP for the packing employed. For random packings, the HETP in extraction will typically range from 0.5 to 1.5 m, depending on the type and size of packing used.

Flooding

No simple correlation is available to predict the flooding velocities in extraction columns, and hence the column diameter needed. The more specialized texts should be consulted to obtain guidance on the appropriate method to use for a particular problem; see Treybal (1980), Green and Southard (2018), and Humphrey and Keller (1997).

17.16.4 Supercritical fluid extraction

A recent development in liquid−liquid extraction has been the use of supercritical fluids as the extraction solvent. Carbon dioxide at high pressure is the most commonly used fluid. It is used in processes for the decaffeination of coffee and tea. The solvent can be recovered from the extract solution as a gas by reducing the pressure. Supercritical extraction processes are discussed by Humphrey and Keller (1997).

17.17 Capital cost of separation columns

Distillation, absorption, and extraction columns are always pressure vessels and must be designed and costed using the methods set out in Chapter 14. Separation columns are often tall structures whose wall thickness can be governed by wind or earthquake loads, so a combined loading analysis is necessary; see Section 14.8. The column diameter and height can be estimated using the methods described in Section 17.11. The maximum design temperature and pressure for the column will usually be calculated from the conditions at the reboiler with a suitable additional margin; see Section 14.4. If the column operates below ambient temperature, then the minimum temperature will be calculated from the condenser temperature with a suitable design margin.

Column internals such as plates or packing are costed separately and added to the vessel cost.

Correlations for preliminary estimates of vessel and internals costs are given in Table 7.2. An example of costing a trayed distillation column is given in Example 7.3.

17.18 References

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17.19 Nomenclature

		Dimensions in MLT θ
A_a	Active area of plate	$\mathbf{L}^2$
A_{ap}	Clearance area under apron	$\mathbf{L}^2$
A_c	Total column cross-sectional area	$\mathbf{L}^2$
A_d	Downcomer cross-sectional area	$\mathbf{L}^2$
A_h	Total hole area	$\mathbf{L}^2$
A_i	Absorption factor	—
A_m	Area term in equation 17.60	$\mathbf{L}^2$
A_n	Net area available for vapor-liquid disengagement	$\mathbf{L}^2$
A_p	Perforated area	$\mathbf{L}^2$
a	Packing surface area per unit volume	$\mathbf{L}^{-1}$
a_w	Effective interfacial area of packing per unit volume	$\mathbf{L}^{-1}$
B	Moles of bottom product per unit time	$\mathbf{MT}^{-1}$
b_i	Moles of component i in bottom product	$\mathbf{M}$
C_o	Orifice coefficient in Equation 17.56	—
C_T	Total molar concentration	$\mathbf{ML}^{-3}$
D	Moles of distillate per unit time	$\mathbf{MT}^{-1}$
D_c	Column diameter	$\mathbf{L}$
D_e	Eddy diffusivity	$\mathbf{L}^2\mathbf{T}^{-1}$
D_L	Liquid diffusivity	$\mathbf{L}^2\mathbf{T}^{-1}$
D_{LK}	Diffusivity of light key component in liquid phase	$\mathbf{L}^2\mathbf{T}^{-1}$
D_v	Diffusivity of vapor	$\mathbf{L}^2\mathbf{T}^{-1}$
d_h	Hole diameter	$\mathbf{L}$
d_i	Moles of component i in distillate per unit time	$\mathbf{MT}^{-1}$
d_p	Size of packing	$\mathbf{L}$
E	Extract flow rate	$\mathbf{MT}^{-1}$
E_a	Actual plate efficiency, allowing for entrainment	—
E_{mV}	Murphree plate efficiency	—
E_{mv}	Murphree point efficiency	—
E_o	Overall column efficiency	—
e	Extract composition	—
FA	Fractional area, equation 17.69	—
F	Feed, of the solution to be extracted	$\mathbf{MT}^{-1}$
F_n	Feed rate to stage n	$\mathbf{MT}^{-1}$
F_p	Packing factor	$\mathbf{L}^{-1}$
F_v	Column "F" factor $= u_a\sqrt{\rho_v}$	$\mathbf{M}^{1/2}\mathbf{L}^{-1/2}\mathbf{T}^{-1}$
F_{LV}	Column liquid−vapor factor in Fig. 17.34	—

		Dimensions in MLT θ
F	Feed composition (in extraction)	—
F	Fractional approach to flooding $= u_a / u_{af}$	—
f_i	Moles of component i in feed per unit time	$\mathbf{MT}^{-1}$
f_1	Viscosity correction factor in Equation 17.79	—
f_2	Liquid density correction factor in Equation 17.79	—
f_3	Surface tension correction factor in Equation 17.79	—
G_m	Molar flow rate of gas per unit area	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$
g	Gravitational acceleration	$\mathbf{LT}^{-2}$
H	Specific enthalpy of vapor phase	$\mathbf{L}^2\mathbf{T}^{-2}$
$\mathbf{H}_G$	Height of gas film transfer unit	$\mathbf{L}$
$\mathbf{H}_L$	Height of liquid film transfer unit	$\mathbf{L}$
$\mathbf{H}_{OG}$	Height of overall gas phase transfer unit	$\mathbf{L}$
$\mathbf{H}_{OL}$	Height of overall liquid phase transfer unit	$\mathbf{L}$
$\mathcal{H}$	Henry's constant	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
h	Specific enthalpy of liquid phase	$\mathbf{L}^2\mathbf{T}^{-2}$
h_{ap}	Apron clearance	$\mathbf{L}$
h_b	Height of liquid backed-up in downcomer	$\mathbf{L}$
h_{bc}	Downcomer back-up in terms of clear liquid head	$\mathbf{L}$
h_d	Dry plate pressure drop, head of liquid	$\mathbf{L}$
h_{dc}	Head loss in downcomer	$\mathbf{L}$
h_f	Specific enthalpy of feed stream	$\mathbf{L}^2\mathbf{T}^{-2}$
h_L	Liquid hold-up on tray	$\mathbf{L}$
h_{ow}	Height of liquid crest over downcomer weir	$\mathbf{L}$
h_r	Plate residual pressure drop, head of liquid	$\mathbf{L}$
h_t	Total plate pressure drop, head of liquid	$\mathbf{L}$
h_w	Weir height	$\mathbf{L}$
K	Equilibrium constant	—
K_G	Overall gas phase mass transfer coefficient	$\mathbf{L}^{-1}\mathbf{T}$
K_i	Equilibrium constant for component i	—
K_L	Overall liquid phase mass transfer coefficient	$\mathbf{LT}^{-1}$
K_1	Constant in Equation 17.49	$\mathbf{LT}^{-1}$
K_2	Constant in Equation 17.52	—
K_3	Percentage flooding factor in Equation 17.80	—
K_4	Parameter in Fig. 17.54, defined by Equation 17.81	—
K_5	Constant in Equation 17.84	—
k_G	Gas film mass transfer coefficient	$\mathbf{L}^{-1}\mathbf{T}$
k_L	Liquid film mass transfer coefficient	$\mathbf{LT}^{-1}$
L	Liquid flow rate, mols per unit time	$\mathbf{MT}-1$
L_m	Molar flow rate of liquid per unit area	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$

		Dimensions in MLT θ
L_p	Volumetric flow rate across plate divided by average plate width	$\mathbf{L^2T^{-1}}$
L_w	Liquid mass flow rate	$\mathbf{MT^{-1}}$
L_w^*	Liquid mass flow rate per unit area	$\mathbf{MT^{-2}T^{-1}}$
L_{wd}	Liquid mass flow rate through downcomer	$\mathbf{MT^{-1}}$
l_h	Weir chord height	**L**
l_p	Pitch of holes (distance between centers)	**L**
l_t	Plate spacing in column	**L**
l_w	Weir length	**L**
M	Number of pure products required	—
M_s	Molecular weight of solvent	—
m	Slope of equilibrium line	—
N	Number of components	—
N	Number of stages	—
$\mathbf{N}_G$	Number of gas-film transfer units	—
$\mathbf{N}_L$	Number of liquid-film transfer units	—
N_{min}	Number of stages at total reflux	—
$\mathbf{N}_{OG}$	Number of overall gas-phase transfer units	—
$\mathbf{N}_{OL}$	Number of overall liquid-phase transfer units	—
N_r	Number of equilibrium stages above feed	—
N_s	Number of equilibrium stages below feed	—
n	Stage number	—
P	Total pressure	$\mathbf{ML^{-1}T^{-2}}$
ΔP_t	Total plate pressure drop	$\mathbf{ML^{-1}T^{-2}}$
p	Partial pressure	$\mathbf{ML^{-1}T^{-2}}$
q	Heat to vaporize one mol of feed divided by molar latent heat	—
q_b	Heat supplied to reboiler	$\mathbf{ML^2T^{-3}}$
q_c	Heat removed in condenser	$\mathbf{ML^2T^{-3}}$
q_n	Heat supplied to or removed from stage n	$\mathbf{ML^2T^{-3}}$
R	Universal gas constant	$\mathbf{L^2T^{-2}}2\theta^{-1}$
R	Reflux ratio	—
R	Raffinate flow rate (in extraction)	$\mathbf{MT^{-1}}$
R_{min}	Minimum reflux ratio	—
r	Raffinate composition	—
S	Extracting solvent flow rate	$\mathbf{MT^{-1}}$
S_i	Stripping factor	—
S_n	Side stream flow from stage n	$\mathbf{MT^{-1}}$
s	Solvent composition	—
t_L	Liquid contact time	**T**

		Dimensions in MLT θ
t_r	Residence time in downcomer	**T**
$\bar{t}_v$	Average vapor residence time	**T**
u_a	Vapor velocity based on active area	$\mathbf{LT}^{-1}$
u_{af}	Vapor velocity at flooding point based on active area A_a	$\mathbf{LT}^{-1}$
u_f	Vapor velocity at flooding point based on net area A_n	$\mathbf{LT}^{-1}$
u_h	Vapor velocity through holes	$\mathbf{LT}^{-1}$
u_n	Vapor velocity based on net cross-sectional area	$\mathbf{LT}^{-1}$
u_v	Superficial vapor velocity (based on total cross-sectional area)	$\mathbf{LT}^{-1}$
V	Vapor flow rate mols per unit time	$\mathbf{MT}^{-1}$
V_w	Vapor mass flow rate	$\mathbf{MT}^{-1}$
V_w^*	Vapor mass flow rate per unit area	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$
x	Mol fraction of component in liquid phase	—
x_b	Mol fraction of component in bottom product	—
x_d	Mol fraction of component in distillate	—
x_e	Equilibrium mol fraction in liquid phase	—
x_i	Mol fraction of component i	—
x_r	Mol fraction of reference component (Equation 17.25)	—
x_1	Mol fraction of solute in solution at column base	—
x_2	Mol fraction of solute in solution at column top	—
x_α	Mol fraction in first liquid phase	—
x_β	Mol fraction in second liquid phase	—
y	Mol fraction of component in vapor phase	—
y_e	Equilibrium mol fraction in vapor phase	—
y_i	Mol fraction of component i	—
Δy	Concentration driving force in the gas phase	—
Δy_{lm}	Log mean concentration driving force	—
y_1	Concentration of solute in gas phase at column base	—
y_2	Concentration of solute in gas phase at column top	—
Z	Height of packing	**L**
Z_c	Liquid hold-up on plate	**L**
Z_L	Length of liquid path	**L**
z_i	Mol fraction of component i in feed stream	—
z_f	Mol fraction of component in feed stream	—
α	Relative volatility	—
α_i	Relative volatility of component i	—
α_a	Average relative volatility of light key	—
θ	Root of Equation 17.29	—

		Dimensions in MLT θ
μ	Dynamic viscosity	$\mathbf{ML^{-1}T^{-1}}$
μ_a	Molar average liquid viscosity	$\mathbf{ML^{-1}T^{-1}}$
μ_s	Viscosity of solvent	$\mathbf{ML^{-1}T^{-1}}$
μ_w	Viscosity of water at 20 °C	$\mathbf{ML^{-1}T^{-1}}$
ρ	Density	$\mathbf{ML^{-3}}$
ρ_s	Density of solvent	$\mathbf{ML^{-3}}$
ρ_w	Density of water at 20 °C	$\mathbf{ML^{-3}}$
σ	Surface tension	$\mathbf{MT^{-2}}$
σ_c	Critical surface tension for packing material	$\mathbf{MT^{-2}}$
σ_w	Surface tension of water at 20 °C	$\mathbf{MT^{-2}}$
Φ	Intercept of operating line on Y axis	—
Φ_n	Factor in Equation 17.80	—
ψ	Fractional entrainment	—
ψ_h	Factor in Equation 17.79	—
Dg	Surface tension number	
Pe	Peclet number	
Re	Reynolds number	
Sc	Schmidt number	
Subscripts		
b	Bottoms	
d	Distillate (Distillate)	
e	At equilibrium with the other phase	
f	Feed	
HK	Heavy key	
l	Component number	
L	Liquid	
LK	Light key	
m	Last stage (in extraction)	
min	Minimum	
n	Stage number	
r	Reference component	
s	Solvent	
v	Vapor	
w	Water	
α	First liquid phase	
β	Second liquid phase	
1	Base of packed column	
2	Top of packed column	
Superscripts		
$'$	Stripping section of column	

17.20 Problems

All of the problems in this chapter can be solved using either hand calculations or process simulation programs. Where data are given, they can be used to confirm the validity of the phase equilibrium model used in a simulation.

17.1. At a pressure of 10 bar, determine the bubble and dew point of a mixture of hydrocarbons, composition, mol%: n-butane 21, n-pentane 48, n-hexane 31. The equilibrium K factors can be estimated using the De Priester charts in Dadyburjor (1978) or found using a process simulation program.

17.2. The feed to a distillation column has the following composition: mol%: propane 5.0, isobutane 15, n-butane 25, isopentane 20, n-pentane 35. The feed is pre-heated to a temperature of 90 °C, at 8.3 bar pressure. Estimate the proportion of the feed that is vapor.

17.3. Propane is separated from propylene by distillation. The compounds have close boiling points, and the relative volatility will be low. For a feed composition of 10% w/w propane, 90% w/w propylene, estimate the number of theoretical plates needed to produce propylene overhead with a minimum purity of 99.5 mol%. The column will operate with a reflux ratio of 20. The feed will be at its boiling point. Take the relative volatility as constant at 1.1.

17.4. The composition of the feed to a debutanizer is given here. Make a preliminary design for a column to recover 98% of the n-butane overhead and 95% of the isopentane from the column base. The column will operate at 14 bar, and the feed will be at its boiling point. Use the shortcut methods and follow the procedure set out below. Use the De Priester charts in Dadyburjor (1978) to determine the relative volatility if solving by hand. The liquid viscosity can be estimated using the data given in Appendix C (available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793).

a. Investigate the effect of reflux ratio on the number of theoretical stages.
b. Select the optimum reflux ratio.
c. Determine the number of stages at this reflux ratio.
d. Estimate the stage efficiency.
e. Determine the number of real stages.
f. Estimate the feed point.
g. Estimate the column diameter.

Feed composition:

		kg/h
propane	C_3	910
isobutane	i-C_4	180
n-butane	n-C_4	270
isopentane	i-C_5	70
normal pentane	n-C_5	90
normal hexane	n-C_6	20

17.5. In a process for the manufacture of acetone, acetone is separated from acetic acid by distillation. The feed to the column is 60 mol% acetone, the balance acetic acid.
The column is to recover 95% of the acetone in the feed with a purity of 99.5 mol% acetone. The column will operate at a pressure of 760 mmHg, and the feed will be pre-heated to 70 °C.
For this separation, determine:

a. The number of minimum number of stages required
b. The minimum reflux ratio
c. The number of theoretical stages for a reflux ratio 1.5 times the minimum
d. The number of actual stages if the plate efficiency can be taken as 60%

Equilibrium data for the system acetone−acetic acid, at 760 mmHg, mol fractions acetone:

liquid phase	0.10	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Vapor phase	0.31	0.56	0.73	0.84	0.91	0.95	0.97	0.98	0.99
Boiling point °C	103.8	93.1	85.8	79.7	74.6	70.2	66.1	62.6	59.2

Reference: Othmer (1943).

17.6. In the manufacture of absolute alcohol by fermentation, the product is separated and purified using several stages of distillation. In the first stage, a mixture of 5 mol% ethanol in water, with traces of acetaldehyde and fusel oil, is concentrated to 50 mol%. The concentration of alcohol in the wastewater is reduced to less than 0.1 mol%.
Design a sieve plate column to perform this separation for a feed rate of 10,000 kg/h. Treat the feed as a binary mixture of ethanol and water.
Take the feed temperature as 20 °C. The column will operate at 1 atmosphere.
Determine:

a. The number of theoretical stages
b. An estimate of the stage efficiency
c. The number of actual stages needed

Design a suitable sieve plate for conditions below the feed point.

Equilibrium data for the system ethanol−water, at 760 mmHg, mol fractions ethanol:

liquid phase	0.019	0.072	0.124	0.234	0.327	0.508	0.573	0.676	0.747	0.894
vapor phase	0.170	0.389	0.470	0.545	0.583	0.656	0.684	0.739	0.782	0.894
Boiling point°C	95.5	89.0	85.3	82.7	81.5	79.8	79.3	78.7	78.4	78.2

Reference: Carey and Lewis (1932).

17.7. In the manufacture of methyl ethyl ketone from butanol, the product is separated from unreacted butanol by distillation. The feed to the column consists of a mixture of 0.90 mol fraction MEK and 0.10 mol fraction 2-butanol, with a trace of trichloroethane.
The feed rate to the column is 20 kmol/h and the feed temperature 35 °C. The specifications required are top product 0.99 mol fraction MEK and bottom product 0.99 mol fraction butanol.
Design a column for this separation. The column will operate at essentially atmospheric pressure. Use a reflux ratio 1.5 times the minimum.
a. Determine the minimum reflux ratio
b. Determine the number of theoretical stages
c. Estimate the stage efficiency
d. Determine the number of actual stages needed
e. Design a suitable sieve plate for conditions below the feed point

Equilibrium data for the system MEK −2-butanol, mol fractions MEK:

liquidphase	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Vapor phase	0.23	0.41	0.53	0.64	0.73	0.80	0.86	0.91	0.95
boiling point °C	97	94	92	90	87	85	84	82	80

17.8. A column is required to recover acetone from an aqueous solution. The feed contains 5 mol% acetone. A product purity of 99.5% w/w is required, and the effluent water must contain less than 100 ppm acetone.

The feed temperature will range from 10 to 25 °C. The column will operate at atmospheric pressure. For a feed of 7500 kg/h, compare the designs for a sieve plate and packed column for this duty. Use a reflux ratio of 3. Compare the capital and utility cost for the two designs.
No reboiler is required for this column; live steam can be used.
Equilibrium data for the system acetone–water is given in Example 17.2.

17.9. In the manufacture of methyl ethyl ketone (MEK), the product MEK is extracted from a solution in water using 1,1,2 trichloroethane as the solvent.
For a feed rate 2000 kg/h of solution, composition 30% w/w MEK, determine the number of stages required to recover 95% of the dissolved MEK using 700 kg/h TCE, with countercurrent flow.
Tie-line data for the system MEK–water–TCE percentages w/w, from Newman et al. (1949).

Water-rich phase		Solvent-rich phase	
MEK	TCE	MEK	TCE
18.15	0.11	75.00	19.92
12.78	0.16	58.62	38.65
9.23	0.23	44.38	54.14
6.00	0.30	31.20	67.80
2.83	0.37	16.90	82.58
1.02	0.41	5.58	94.42

17.10. Chlorine is to be removed from a vent stream by scrubbing with a 5% w/w aqueous solution of sodium hydroxide. The vent stream is essentially nitrogen, with a maximum concentration of 5.5% w/w chlorine. The concentration of chlorine leaving the scrubber must be less than 50 ppm by weight. The maximum flow rate of the vent stream to the scrubber will be 4500 kg/h. Design a suitable packed column for this duty. The column will operate at 1.1 bar and ambient temperature. If necessary, the aqueous stream may be recirculated to maintain a suitable wetting rate.
Note: The reaction of chlorine with the aqueous solution will be rapid, and there will be essentially no back-pressure of chlorine from the solution.

CHAPTER

18

Specification and design of solids-handling equipment

KEY LEARNING OBJECTIVES

- The importance of solids-handling operations in the process industries
- How to size and design equipment for sizing, handling, transporting, mixing, and storing solids
- How to size and design equipment to recover solids from gas and liquid streams
- How to design dryers
- How to design equipment for forming solid particles with the desired shape, size, and properties
- Hazards intrinsic to solids processing

18.1 Introduction

Solid-phase materials are encountered in most chemical processes. Foods, fertilizers, polymers, and most pharmaceutical products are finished as solid-phase products. Minerals, coal, biomass, and recycled materials are solid-phase feeds. Most specialty chemical and pharmaceutical processes use crystallization as a means of achieving high-purity products. Even processes that handle only vapor and liquid streams usually use solid-phase catalysts and adsorbents.

Solids are, in general, more difficult to process than gases or liquids. The equipment used for processing solids consumes more power (electricity) and is more likely to suffer mechanical failure. Solids-handling plants can be prone to shutdowns due to caking or plugging of equipment or interruptions of solids flow caused by bridging of poorly designed hoppers and feeders. Solids can form dusts during processing, which cause safety, industrial hygiene, and environmental hazards that must be carefully controlled and mitigated.

The design of solids-handling plant is rarely given adequate attention in undergraduate chemical engineering courses, and most graduating engineers are only superficially aware of solids-handling operations. A wide range of specialized equipment is used in solids processing, and there can be large differences between different vendors' designs. Although there is insufficient space in this volume to give detailed design principles for all solids-handling operations, the following sections introduce the most commonly encountered unit operations and provide references that go into greater detail. A great deal of additional information can be found by searching manufacturers' websites on the Internet.

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As with all process operations that use proprietary equipment, final equipment selection and costing should always be carried out in consultation with a vendor.

18.2 Properties of granular materials

This section gives an overview of the physical properties of solid materials that affect their handling, flow, and storage behavior and that are important in the design of solids-processing equipment.

A bulk solid is an aggregate of many individual particles. Some processing operations are primarily affected by individual particle properties, whereas others are designed based on properties of the bulk material or distributions of individual particle properties.

Several books have been written on the characterization and classification of particles and powders: Allen (1996, 1997), Merkus (2009), and Stanley-Wood and Lines (1992). These discuss the various measurement techniques used and go into considerably more detail than is needed for most chemical engineering design purposes. Kaye (1997), Rhodes (2008), and Higashitani et al. (2019) provide good overviews of these subjects.

18.2.1 Properties of solid particles

Very few of the solid materials encountered in the process industries consist of uniform dense spheres. Particle properties are affected by the intrinsic properties of the material, as well as the processes by which solid particles are formed, shaped, sized, and handled.

Individual particle properties can be very important for end-use applications and are often required as product specifications for solid products. For example, the size and shape of tablets must be highly uniform to ensure that patients receive the correct dose and release rate of an active pharmaceutical ingredient.

Particle size and shape

Particle size is one of the most important characteristics for processing of solids. The effective particle diameter occurs in the design equations for many types of solids-handling equipment. Unfortunately, for irregular-shaped particles there is no simple definition of the effective diameter, and different definitions may be most suitable in different circumstances.

An irregular particle can be characterized in several ways. Consider Fig. 18.1. If the particle is lying flat in a stable position, the longest dimension is obvious and is defined as the length, L. The dimension in the direction perpendicular to the longest axis in the plane of stability is defined as the width, W, and the dimension in the direction normal to the plane of stability is defined as the thickness, t.

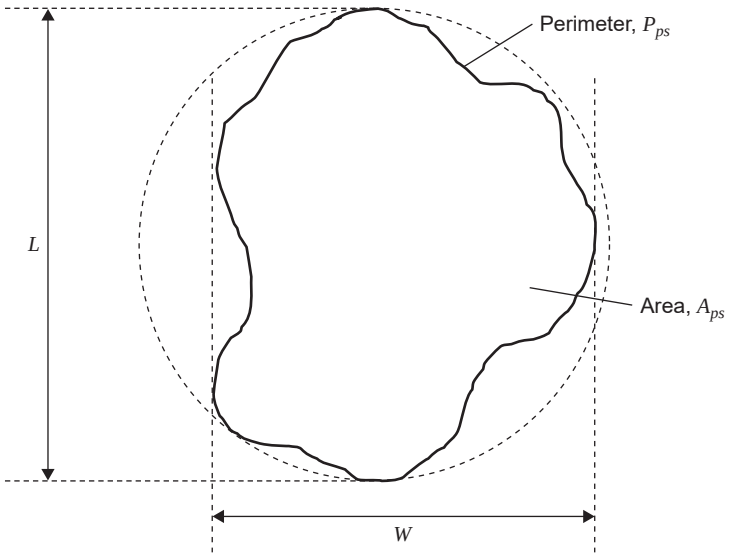


FIG. 18.1 Characterization of an irregular-shaped particle.

The ratio *L/W* is called the elongation or aspect ratio. Particles with elongation greater than 3.0 are often classified as fibers. The inverse of elongation is known as the *chunkiness*, which is often used in preference to elongation, as it necessarily varies between 0 and 1.0 and so is easier to use when plotting graphs. The ratio *W/t* is known as the *flakiness* factor. Particles with high flakiness can be difficult to filter and flow out of hoppers due to their tendency to stack.

The diameter of a circle that has the same projected area as the particle is:

$$d_a = 2\sqrt{\frac{A_{ps}}{\pi}} \tag{18.1}$$

where:

d_a = diameter of a circle with same projected area as the particle
A_{ps} = projected area of the particle

A circle with the same perimeter as the particle would have diameter d_{pr}, given by:

$$d_{pr} = \frac{P_{ps}}{\pi} \tag{18.2}$$

where:

P_{ps} = perimeter of the particle

The conventional definition of the effective hydraulic diameter, d_h, is four times the area divided by the wetted perimeter:

$$d_h = \frac{4\ A_{ps}}{P_{ps}} \tag{18.3}$$

The Stokes diameter, d_{st}, is defined as the diameter of a smooth sphere of the same density as the particle that settles at the same velocity in a viscous liquid.

The *sphericity* of a particle, Ψ, can be defined as:

$$\Psi = \frac{\text{Surface area of a sphere with the same volume as the particle}}{\text{Surface area of the particle}} \tag{18.4}$$

Depending on the physical basis of the method used, different measurement techniques will measure different dimensions as the effective "diameter." For example, for sieves, screens, and filters, the governing dimension is the width, *W*. Sedimentation and elutriation methods will measure the Stokes diameter, d_{st}. Optical analysis by microscopy will measure the area, A_{ps}, and hence d_a. Methods have been developed to relate d_{st} to optical or sieve measurements; see, for example, Heywood (1961).

Screening results are usually given in terms of screen mesh sizes. Different standard mesh sizes are used in the United States and internationally. Table 18.1 gives the dimensions corresponding to different standard wire mesh sieve sizes.

Density and porosity

The density of particulate materials can also be difficult to measure due to the presence of internal pores, cracks, and imperfections in the particles.

The *true density*, also known as *framework*, *crystalline*, or *structural* density, is defined as the density of the material from which the particles are constituted. The *apparent density*, *piece density*, or *particle density* is the observed density of the particles allowing for internal porosity within a particle. The *bulk density* is the density of a large collection of particles, which is further reduced because of the presence of void space between particles.

The bulk density is related to the apparent density and bed void fraction, ε:

$$\rho_b = \rho_p(1-\varepsilon) \tag{18.5}$$

where:

ρ_b = bulk density
ρ_p = particle density
ε = bed void fraction

TABLE 18.1 Standard wire mesh sieve sizes

ASTM (E-11)	Tyler equivalent	Sieve opening (mm)	Sieve opening (in)
100 mm		100.0	~4.00
75 mm		75.0	~3.00
50 mm		50.0	~2.00
25 mm		25.0	~1.00
12.5 mm		12.5	~0.50
6.3 mm		6.3	~0.25
No. 4	**4 mesh**	4.75	0.187
No. 5	**5 mesh**	4.00	0.157
No. 6	**6 mesh**	3.35	0.132
No. 7	**7 mesh**	2.80	0.110
No. 8	**8 mesh**	2.36	0.0937
No. 10	9 mesh	2.00	0.0787
No. 12	10 mesh	1.70	0.0661
No. 14	12 mesh	1.40	0.0555
No. 16	14 mesh	1.18	0.0469
No. 18	16 mesh	1.00	0.0394
No. 20	**20 mesh**	0.85	0.0331
No. 25	24 mesh	0.71	0.0278
No. 30	28 mesh	0.60	0.0234
No. 35	32 mesh	0.500	0.0197
No. 40	35 mesh	0.425	0.0165
No. 45	42 mesh	0.355	0.0139
No. 50	48 mesh	0.300	0.0117
No. 60	**60 mesh**	0.250	0.0098
No. 70	65 mesh	0.212	0.0083
No. 80	**80 mesh**	0.180	0.0070
No. 100	**100 mesh**	0.150	0.0059
No. 120	115 mesh	0.125	0.0049
No. 140	150 mesh	0.106	0.0041
No. 200	**200 mesh**	0.075	0.0029
No. 400	**400 mesh**	0.038	0.0015

S.I. units are ASTM standard. 25.4 mm = 1.00 in.
Values in bold are those for which the ASTM designations and Tyler equivalent series match.

Similarly, the particle density is related to the true density and the internal porosity (internal pore volume fraction), χ:

$$\rho_p = \rho_t(1-\chi) \tag{18.6}$$

where:

ρ_t = true density
χ = internal pore volume fraction

The density of a fully wetted particle in a fluid of density ρ_f is:

$$\rho_w = \rho_p + \rho_f \chi \tag{18.7}$$

where:

ρ_w = wetted particle density

If a container of known volume is filled with particles and weighed, then the bulk density can be calculated. Adding a liquid that fills the interparticle voids but does not fill the internal cracks and pores allows measurement of the particle external volume and hence the apparent density. Adding a liquid that fills the internal cracks and pores or measuring the gas volume added to achieve a given change in pressure similarly allows measurement of the particle framework volume and hence the true density.

Bulk density is highly sensitive to packing of the particles and can be increased by tapping or compacting the bed, particularly for fine powders or materials with high flakiness. A compacted bed will typically have 5% to 20% higher density than an uncompacted bed. Typical values of bulk density are given in Table 18.2.

In most design situations, the apparent density is used for individual particles and the average bulk density is used for sizing fixed beds, bins, hoppers, and conveyors. The apparent density is valid for dry particles in gas flows and for particles that are wetted by a surrounding fluid. The wetted density should be used when a wet particle is surrounded by a gas (as in a dryer) to allow for the liquid in the pores. An initial estimate of particle density can often be made by assuming a typical value of 0.4 for the bed void fraction in Equation 18.5.

The internal porosity of particles is very important in many applications. Internal porosity greatly increases the surface area of the particles, increasing the rate of dissolution in a solvent and providing additional surface area for adsorption, reaction, or catalysis. Because the internal surface area is usually more important than the fraction of internal volume occupied by pores, porosity is often expressed as surface area per unit mass, typically given in m^2/g. Internal surface area is measured by gas adsorption studies; see Allen (1996).

Particle strength and hardness

The strength of individual particles of a granular material depends on the material from which the particles are made, as well as the microstructure of the particles. Many solid products are actually composites or agglomerates, formed by binding smaller particles together in a matrix of liquid or solid binder. The strength of agglomerates depends on the chemical and physical nature of the binder; see Pietsch (1997). The use of agglomeration to increase particle size is discussed in Section 18.8.

Particle strength is an important property of formed particles such as pharmaceutical tablets, catalyst pellets, and processed foods such as candies and breakfast cereals. Formed particles must be strong enough to survive processing during manufacture as well as end-use requirements. Catalyst pellets must be strong enough to withstand the forces exerted on them when loaded into a fixed bed or the impacts encountered in fluidized-bed or moving-bed reactors. Tablets must often be designed to be strong enough to keep their shape during packaging and shipping but weak enough to be easily split in two by the patient or caregiver. Formed foods such as breakfast cereals and baked snacks must have sufficient strength to be crunchy but not be so strong that the consumer breaks their teeth.

Particle strength is often confused with hardness, although they are not strictly related except for particles that are microscopically homogeneous and free from defects. Hardness is defined as a measure of the ability of a material to scratch or wear another material. Hardness is a good predictor of how abrasive a material will be and hence how rapidly it will cause wear or erosion of contacting surfaces such as cyclones or grinding equipment. The grindability of a nonuniform solid depends more on the particle strength than the hardness. For example, small inclusions of quartz in raw minerals can make the material very abrasive without making it resistant to crushing or grinding. Hardness is typically measured on the Moh hardness scale. The Moh hardness scale is a relative ranking of hardness ranging from 1 (talc) to 10 (diamond), where materials are ranked based on their scratch test performance relative to other materials. The Moh hardness scale is given in Fig. 18.69 in the discussion of grinding in Section 18.9. Values of Moh hardness for some common materials are given in Table 18.2.

The strength of individual particles is usually stated as the *crush strength*, which is the resistance to compression measured in a load cell. Standard methods for measuring particle crush strength are ASTM D6175 and ASTM D4179. The particle crush strength is sometimes referred to as *piece crush strength*. Values of crush strength are conventionally reported as the average force in lb_f required to break a particle. In some cases, specifications are set on the standard deviation as well as the mean crush strength of the product.

TABLE 18.2 Typical properties of particulate materials

Material	Average bulk density (kg/m^3)	Moh Hardness	Angle of repose, β (degrees)	Bond work index (kWh/2000 lb)
Alumina beads	2050	2	34	
Ash, dry fly ash	610	1	40	
Bauxite	1090	5	31	9.45
Calcium oxide	430		43	
Carbon	800	1	21	
Catalyst, 100 micron FCC	510	2	32	
Cement, Portland	1520		39	10.5
Clay, kaolin, crushed	1025		35	7.1
Coal, bituminous, dry	670	2	29	11.4
Coal, bituminous, wet	800	2	40	
Coffee beans	670		25	
Coke, petroleum	640	2	34	73.8
Corn, shelled	720	1	21	
Dolomite, crushed	740	4	41	11.3
Glass beads, 280 micron	1500	7	26	
Gypsum, ground	900	2	40	8.16
Lead shot, 0.25 in.	6600	1	33	
Lime, burned and pulverized	430	3	43	
Limestone, coarse	1570	4	25	11.6
Mica, ground	220		36	135
Phosphate, dicalcium	960		30	
Phosphate rock	960	4	40	10.1
Phthalic anhydride, flakes	670	1	24	
Rice	800		20	
Rubber, ground tire	370		35	
Salt, granulated	1300	2	31	
Sand, coarse	1500	7	30	16.5
Sand, very fine	1500	7	32	
Sawdust	320	1	45	

Soap powder	160	1	30
Soda ash, light	480	1	37
Sodium nitrate	1090		24
Soybeans	770	1	39
Sulfur powder	800	3	45
Wheat	770	1	23
Wood chips	350		36

Notes:

1 Adapted from data in Zenz and Othmer (1960) and Green and Southard (2018).
2 Average bulk densities can vary ±10%

The strength of an aggregate of particles is not the same as the strength of an individual particle and can be measured using ASTM method D7084. The strength of bulk minerals is more often reported as a *work index*, which is a measure of the difficulty of grinding the material. The work index is defined and described in Section 18.9.

An important property related to particle strength is attrition resistance, which is a measure of how easily smaller particles can be broken off from the surface of a larger particle. Particles that are easily reduced to smaller particles by friction or that crumble under low pressures are described as *friable* and tend to form dust during transport, handling, processing, and storage. Many hazards are associated with dust formation (see Section 18.11), so special care must be taken when designing plant for friable solids. The attrition resistance of formed products can be measured using the methods described in ASTM D4058.

Particle chemical properties

Chemical properties of the material of which particles are composed can have a strong influence on particle density, porosity, and strength or can introduce health and safety hazards that affect processing. Chemical reactions can also lead to changes in these properties, particularly when particles are exposed to air or atmospheric moisture.

Solid materials that are toxic, corrosive, combustible, or explosive must be handled with particular care. Hazards of processing solids are described in Section 18.11. Materials that would normally be considered inert can become extremely hazardous during processing, for example, if they become saturated with a flammable solvent or if grinding or abrasion exposes an unoxidized surface that can react with air.

Many solid materials are hygroscopic and will absorb water if exposed to ambient air. This affects the particle density and can also affect particle strength. Many minerals have a different crystalline structure in the hydrated state. Moisture content can also dramatically change the bulk flow properties of granular materials; see Armstrong et al. (2014) for examples.

Many solid materials are susceptible to oxidation in air. This can be particularly hazardous during grinding, as fresh surface area will be exposed. Oxidation is an exothermic reaction that can run away and cause ignition of the solids.

Grinding can also cause release of volatile compounds from a solid when fresh surface area is exposed. This can affect the chemical composition of the solids. In many foods, volatile organic compounds (VOCs) play a critical role in determining flavor, and process operations must be designed to reduce loss of these compounds by evaporation. For example, this effect is important in processing of coffee and cacao beans and explains why many consumers prefer to grind coffee close to the point of consumption.

18.2.2 Bulk and flow properties of particulate materials

A bulk mass of particles has some characteristics that are aggregate properties of the individual particles, as well as properties that depend on interparticle interactions. The properties of bulk solids are strongly dependent on the distribution of particle size and can also vary significantly from sample to sample within the same material.

Particle size distribution

All solids streams encountered in the process industries have a distribution of particle sizes. Even narrow-cut screened fractions will have a range of sizes between the upper and lower screen aperture sizes.

In some processes and unit operations the use of a mean "diameter" is sufficient. The choice of dimensions to use as diameter is discussed in Section 18.2.1 and in the sections on each unit operation. Several different mean diameters can also be defined, each of which is most appropriate in given situations. The simplest definitions are the arithmetic and geometric mean diameters:

$$\overline{d_a} = \sum_{i=1}^{N} \frac{d_i}{N} \tag{18.8}$$

$$\overline{d_g} = \left(\prod_{i=1}^{N} d_i \right)^{1/N} \tag{18.9}$$

where:

$\overline{d_a}$ = arithmetic mean diameter
$\overline{d_g}$ = geometric mean diameter
d_i = diameter of particle i
N = number of particles in sample

Many chemical engineering operations involve a balance between phenomena related to area and phenomena related to volume (or mass), so one of the most useful definitions is the volume−surface mean diameter:

$$\overline{d_{vs}} = \frac{\sum_{i=1}^{N} d_i^3}{\sum_{i=1}^{N} d_i^2} \tag{18.10}$$

where:

$\overline{d_{vs}}$ = volume surface mean diameter

Although a mean diameter may be appropriate in many design problems, there are several unit operations that have different outcomes depending on particle size. For these operations, the design engineer must work with a distribution of particle sizes. For example, the efficiency of a cyclone for capturing particles depends strongly on the particle size and will be substantially lower for very fine particles less than 5 μm in diameter.

Particle size distributions are usually discretized and reported as number or mass fractions of particles within a given size range. Care must be taken when reading a particle size distribution to ensure that the fraction stated is over or under the given size.

Commercial process simulation programs usually have the ability to track particle size distribution of solids streams and allow the user to manipulate the particle size distribution in operations such as crystallizers, cyclones, filters, and agglomerators.

Voidage and bulk density

The void fraction (voidage) and average bulk density of a collection of particles were introduced in Section 18.2.1. The bulk density and voidage are related by Equation 18.5.

For fine particles, the void fraction can be a strong function of bed packing. Vibrating or tamping a bed of fine particles causes the particles to settle and reduces the void fraction. For regular-shaped, cohesionless materials with narrow size distribution, the change in bed density is usually in the range of 1% to 10%, but for materials with a wide range of particle size, the density can be increased by up to 40% (Seville et al., 1997). When there is a wide range of particle size, the smaller particles can fit into the spaces between the larger particles, as illustrated schematically in Fig. 18.2, and hence lower voidage is possible.

Compaction or compression of a bed of particles is sometimes desired, for example, when the design calls for maximizing the amount of a solid such as an adsorbent in a given volume. In such cases, the bed is dense loaded and compacted during loading. More often, compaction is not desired but occurs naturally when solids are stored or transported. It can be difficult to initiate free flow from a compacted bed of solids, and the pressure drop is higher when flowing a fluid through a compacted bed because of the lower voidage.

Cohesion

Cohesion is a measure of the tendency of particles to stick together. Cohesion arises from several different particle-to-particle interactions:

1. Van der Waals forces between particles
2. Electrostatic forces between particles
3. Interlocking of irregularly shaped particles
4. Capillary action and surface tension forces due to liquid bridges between particles
5. Forces between adsorbed layers or coatings on particles

Cohesion should not be confused with friction forces between particles that are moving and can be thought of as the force that must be overcome to initiate movement of particles rather than the force to maintain movement.

Cohesive forces tend to be stronger for small particles and particles that are moist or partially wetted, particularly if the liquid has a high surface tension. For example, sand, grain, and sugar have low cohesion when dry, but can be very cohesive when moist. It is the cohesion of wet sand that allows the construction of sand castles with near-vertical walls.

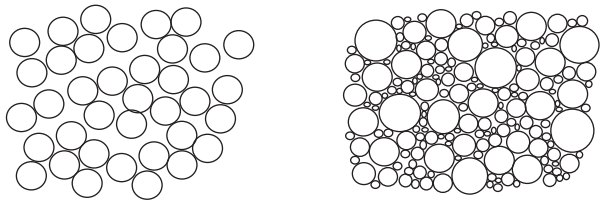


FIG. 18.2 Packing of beds of particles with different size distributions.

Flow properties

Powders and particulate materials can be treated as rigid, semi-plastic, continuous materials for the purposes of modeling flow in bins and hoppers. A rigid, semi-plastic Coulomb solid has a linear yield locus, as shown in Fig. 18.3. If the applied shear stress is greater than the yield locus, slip will occur and the material will flow.

For a Coulomb solid:

$$\tau = c + \sigma \tan \alpha \tag{18.11}$$

where:

τ = shear stress
c = cohesion
σ = normal stress (applied load)
α = angle of internal friction

The angle of internal friction should not be confused with the angle of repose of the solids. The angle of repose, β, is the angle formed by a pile of solids loosely tipped onto a surface (Fig. 18.4). The angle of internal friction can be measured as the angle formed between stationary and flowing material when solids are flowed out from a flat-bottomed slotted vessel (Fig. 18.5). The cohesion and angle of internal friction can also be measured in appropriately designed shear cells; see, for example, Thomson (1997). Some examples of angle of repose are given in Table 18.2.

The angle of internal friction can be affected by packing density and consolidation. The angle of internal friction tends to be lower for materials that are dry and have small particles and higher for materials that are cohesive, are moist, or contain large particles.

When a Coulomb material is placed on an inclined surface, the friction between the solid and the wall can be less than the internal friction, causing the material to slide down the wall. If there are no cohesive forces between the material and the wall, then a wall yield locus can be defined:

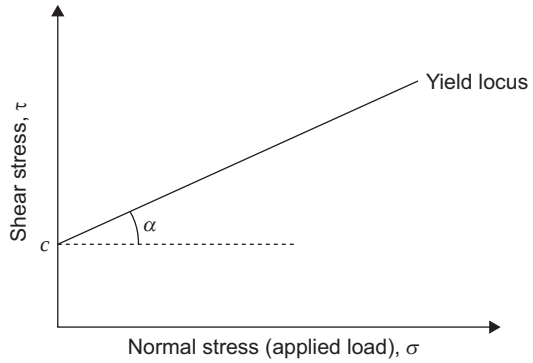


FIG. 18.3 Yield locus of a bed of solid particles.

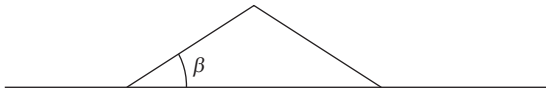


FIG. 18.4 Angle of repose of a pile of solid particles.

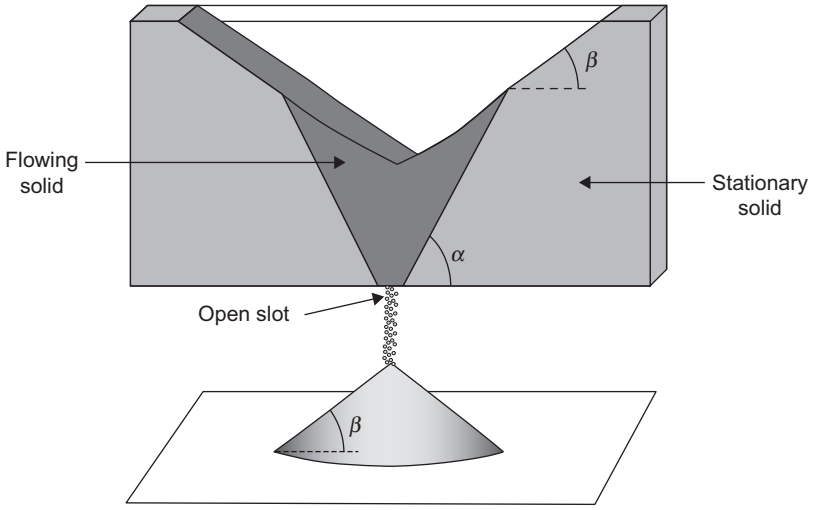


FIG. 18.5 Measuring the angle of internal friction and angle of repose.

$$\tau_w = \sigma_w \tan \alpha_w \tag{18.12}$$

where:

τ_w = shear stress at the wall
σ_w = normal stress at the wall
α_w = angle of wall friction

The angle of wall friction can be measured as the slope of a surface along which particles will slide (Fig. 18.6).

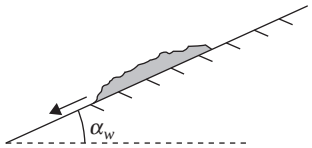


FIG. 18.6 Angle of wall friction.

Fluidization

The pressure drop of a fluid flowing through a bed of granular solids can be estimated using the Ergun equation (Ergun, 1952):

$$\frac{\Delta P}{L_b} = 150\frac{(1-\varepsilon)^2}{\varepsilon^3}\frac{\mu U}{d_p^2} + 1.75\frac{(1-\varepsilon)}{\varepsilon^3}\frac{\rho_f U^2}{d_p} \tag{18.13}$$

where:

ΔP = pressure drop, N/m^2
L_b = length of the bed of solids, m
ε = void fraction
μ = fluid viscosity, Ns/m^2
U = fluid superficial velocity, m/s
d_p = particle effective diameter, m
ρ_f = fluid density, kg/m^3

If the fluid flows upwards, then at some point the force due to pressure drop balances the weight of the particles and the bed begins to expand and become fluidized (Fig. 18.7b). As the fluid flow rate increases, the bed expands further and can enter bubbling, slugging, or spouting regimes, illustrated in Figs. 18.7(c) and (d). If the fluid flow is increased to the point where the superficial velocity is equal to the terminal velocity of the smallest particles, these particles are elutriated from the bed and carried out with the fluid. Ultimately, at high enough velocities, the entire bed can be entrained into the fluid flow, and pneumatic or hydraulic conveying of the particles occurs.

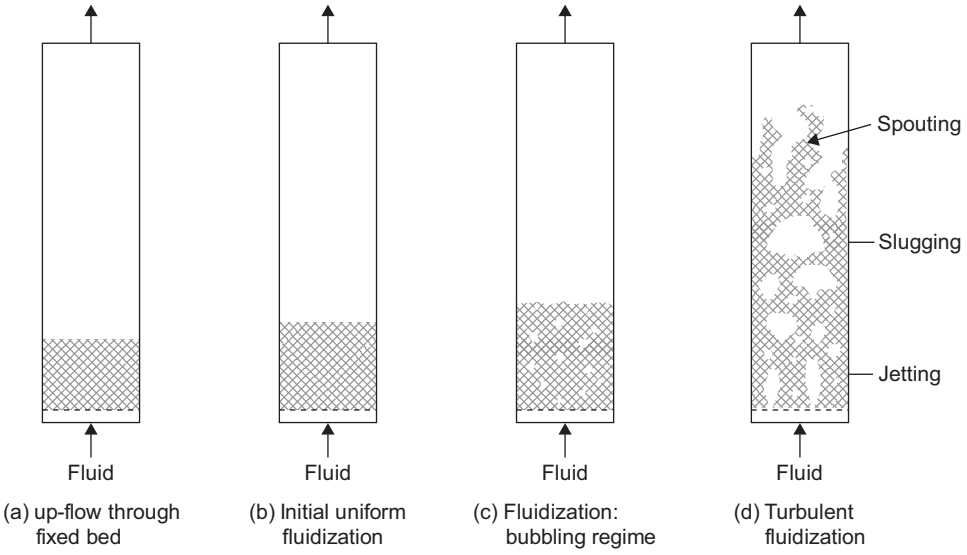


FIG. 18.7 Fluidization of a bed of particles.

The onset of fluidization can be predicted by balancing the pressure drop against the buoyant weight of the bed:

$$\frac{\Delta P}{L_b} = (1-\varepsilon_{mf})(\rho_p - \rho_f)g \tag{18.14}$$

where:

ε_{mf} = void fraction at minimum fluidization
g = gravitational acceleration, m/s^2
ρ_p = particle density, kg/m^3

Substituting the Ergun equation for pressure drop:

$$(1-\varepsilon_{mf})(\rho_p - \rho_f)g = 150\frac{(1-\varepsilon_{mf})^2}{\varepsilon_{mf}^3}\frac{\mu U_{mf}}{d_p^2} + 1.75\frac{(1-\varepsilon_{mf})}{\varepsilon_{mf}^3}\frac{\rho_f U_{mf}^2}{d_p}$$

where U_{mf} is the superficial fluid velocity at minimum fluidization.
Rearranging:

$$\frac{\rho_f(\rho_p - \rho_f)g\ d_p^3}{\mu^2} = 150\frac{(1-\varepsilon_{mf})}{\varepsilon_{mf}^3}\frac{\rho_f d_p U_{mf}}{\mu} + \frac{1.75}{\varepsilon_{mf}^3}\frac{\rho_f^2 d_p^2 U_{mf}^2}{\mu^2} \tag{18.15}$$

The Reynolds number at minimum fluidization, $\mathbf{Re_{mf}}$, is:

$$\mathbf{Re_{mf}} = \frac{\rho_f d_p U_{mf}}{\mu} \tag{18.16}$$

We can also define the dimensionless Archimedes number, **Ar**:

$$\mathbf{Ar} = \frac{\rho_f(\rho_p - \rho_f)g\ d_p^3}{\mu^2} \tag{18.17}$$

The Archimedes number is a dimensionless volume, and $\mathbf{Ar}^{1/3}$ is a dimensionless diameter. We can then rewrite Equation 18.15 as:

$$\mathbf{Ar} = 150\frac{(1-\varepsilon_{mf})}{\varepsilon_{mf}^3}\mathbf{Re_{mf}} + \frac{1.75}{\varepsilon_{mf}^3}\mathbf{Re_{mf}^2} \tag{18.18}$$

This is not particularly useful if we have no knowledge or measurement of ε_{mf}, but Wen and Yu (1966) correlated a large set of data to obtain:

$$\mathbf{Ar} = 1650\ \mathbf{Re_{mf}} + 24.5\ \mathbf{Re_{mf}^2} \tag{18.19}$$

Note that although the Wen and Yu correlation has the same form as Equation 18.18, it does not yield a unique value for ε_{mf}.

The different types of fluidization behaviors can be plotted on a graph of dimensionless superficial velocity versus dimensionless diameter ($\mathbf{Ar}^{1/3}$), as shown in Fig. 18.8, which is taken with permission from Grace (1986). It can be seen that conventional fluidized beds are usually stable over about an order of magnitude of superficial velocity before turbulence and elutriation begin, although this is obviously somewhat sensitive to the particle size distribution. The classification of particles as Groups A, B, C, and D refers to the system developed by Geldart (1973), summarized in Table 18.3. For more detail on prediction of different fluidization regimes, see Seville et al. (1997), Zenz and Othmer (1960), or Zenz (1997).

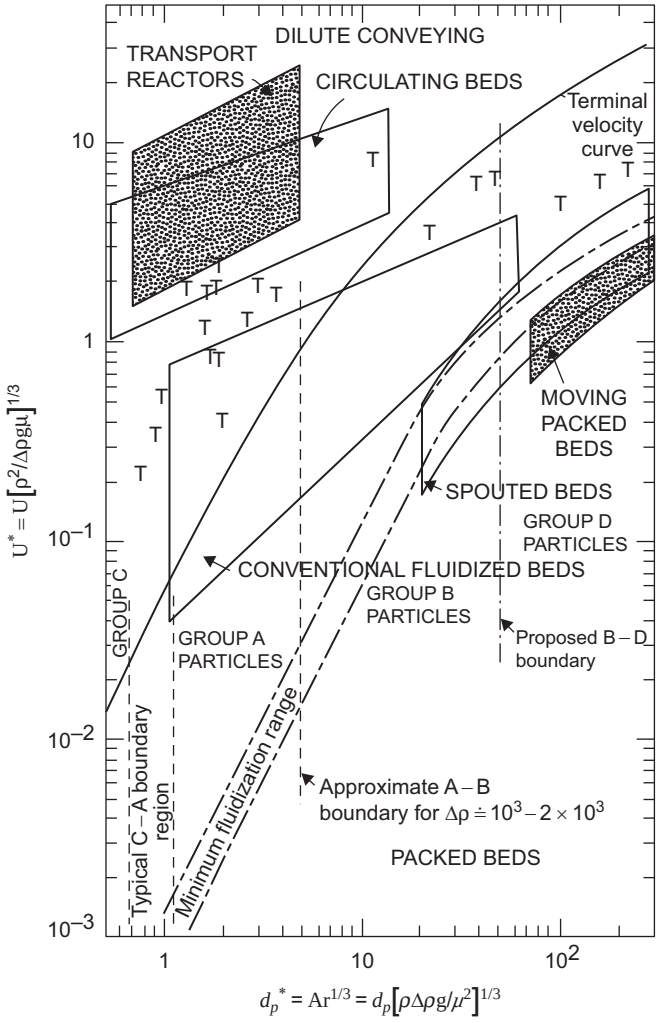


FIG. 18.8 Fluidization regimes. *Taken, with permission, from Grace, J. R. (1986). Contacting modes and behavior classification of gas-solid and other two-phase suspensions,* Canadian Journal of Chemical Engineering, 64*(3), 353. "T" indicates experimentally observed onset of turbulent fluidization.*

Most fluidized beds are operated under conditions where they are well-mixed in the solids phase and have very uniform temperature. They have high rates of heat transfer to internal and external surfaces, as heat is effectively carried and transferred by the solid particles. The uniform temperature and high heat transfer experienced in fluidized beds can be advantageous for carrying out reactions. Fluidized beds can also be used to transport heat from a hot zone such as a regeneration reactor to an endothermic reactor, as occurs in catalytic cracking; see Section 15.8.4.

TABLE 18.3 Geldart's classification of fluidization behavior

Group	C	A	B	D
Major characteristic	Cohesive Hard to fluidize	Bubble-free over some range	Bubbles at U_{mf}	Coarse solids
Bed expansion	Low, prone to Channeling	High	Moderate	Low
Bubble behavior	Channels	Bubbles coalesce to limiting size	Large stable bubbles	Large slugs
Solids mixing	Low	High	Moderate	Low
Gas back-mixing	Low	High	Moderate	Low
Spouting	No	Shallow beds only	Shallow beds only	Yes
Examples	Flour, cement	Cracking catalyst	Sand, salt	Crushed rock, beans

From Geldart (1973).

Fluidized beds also allow easy continuous addition and removal of solids, which can be important in catalytic reactions if the catalyst deactivates.

The main disadvantage of fluidized beds is that attrition can cause erosion of the vessel internals and formation of fine solid particles. Fluidized-bed equipment is often lined with refractory material to prevent erosion of the structural metal. Fluidized beds are usually fitted with cyclones to capture and return larger particles, but secondary or tertiary capture systems may be needed for environmental reasons or to prevent loss of expensive catalyst. Caution is also needed when designing a fluidized bed at higher velocities, particularly for gases, as bubbling or slugging can cause part of the fluid flow to bypass the bed, reducing reaction or heat-transfer efficiency, See Cocco et al. (2014a) for design approaches to address these problems. Solids that have high cohesion or high tendency to agglomerate are usually not suitable for fluidization.

Fluidization is important in several solids-handling and processing operations. Some catalytic reactors are designed to operate as fluidized beds; see Sections 15.7 and 15.8, whereas packed beds that are used in up-flow in reactors or adsorption columns must be designed to avoid fluidization. Fluidization is also used in some designs of solids heaters and dryers, in some agglomerators, and in pneumatic and hydraulic conveying. Fluidized beds are widely used in minerals processing and in the combustion of coal. For more information on fluidization and its applications, see the introductory article by Cocco et al. (2014b) and the books by Zenz and Othmer (1960), Seville et al. (1997), Kunii and Levenspiel (1991), and Yang (1999, 2003).

18.3 Storage and transport of solids

18.3.1 Storage of bulk solids

The simplest way to store raw bulk solids is to pile them on the ground in the open air. This is satisfactory for the long-term storage of materials that do not deteriorate on exposure to the elements, for example, the seasonal stockpiling of coal at mines and power stations. For large stockpiles, permanent facilities are usually installed for distributing and reclaiming the material; traveling gantry cranes, grabs, and drag scrapers feeding belt conveyors are used. For small, temporary storage, mechanical shovels, front-end loaders, and trucks can be used. When the cost of recovery from the stockpile is large compared with the value of the stock held, storage in silos or bunkers should be considered. There is no upper limit to the amount of material that can be stored in open piles, but the design engineer should be concerned about visual impact and the possibility of water run-off contaminating local surface and ground water.

Solids can also be piled inside storage sheds or warehouses. This affords protection from the weather and can be cheaper than using silos for large quantities. Indoor storage is used for stockpiling seasonal products such as fertilizers that are water-soluble and so cannot be stored outside.

Storage bins are used for solids that must be protected from the elements and for storing smaller quantities of solids for process use. A *bin* is any vertical walled vessel used for storing solids. Most bins have a conical or wedge-shaped *hopper* at the base, though some bins are flat-bottomed. Large bins with a height-to-diameter ratio greater than 1.5 are also called *silos*, whereas bins with a height-to-diameter ratio less than 1.5 are termed *bunkers*.

Large bunkers and silos used for agricultural products, cement, and bulk minerals typically hold 50 to 1000 metric tons of solids and are usually constructed from reinforced concrete. The design of large bins requires analysis of the wall stresses caused during filling and discharge of the solids and is beyond the scope of this book; see Fayed and Otten (1997) and Seville et al. (1997). Large-scale concrete silos are often used to store material for days, weeks, or even months.

Smaller bins and silos for handling the feeds to chemical and pharmaceutical processes typically contain less than 10 tons of material and are constructed from steel or glass-reinforced polymer (GRP). Bins and silos for process use are usually sized to contain enough material to ensure correct operation of the feeder device at the base of the hopper (see Section 18.3.2) and to provide adequate residence time to compensate for short interruptions in any upstream system that is feeding the bin. A residence time of 1 to 3 hours is typical, but longer residence times are used when the flow rate is small or when the upstream operation is highly discontinuous. The sizing of a process feed bin is illustrated in Example 18.1.

18.3.2 Discharge from bins and hoppers

Process bins and silos are usually designed to give a uniform flow rate of solids to downstream operations. The flow of solids from a bin or hopper is influenced by the shape of the hopper, the size of the discharge opening, and the use of devices known as *feeders* to regulate the flow.

Flow patterns in bins and hoppers

There are two main types of flow from a bin or hopper, as illustrated schematically in Fig. 18.9. When the wall angle of the hopper is steep enough, mass flow occurs, as illustrated in Fig. 18.9(a). In mass flow, slip occurs between the solids and the wall and all of the particulate material is moving downwards. There are no stagnant regions in the bin or hopper, and there is a reduced tendency for the particles to segregate by particle size during flow. This flow pattern is also known as "first-in-first-out," as material from the top of the bin does not channel to the exit.

If the wall angle of the hopper is not sufficiently steep, or if discharge occurs from an opening at the base of a flat-bottomed bin, then funnel flow occurs, as illustrated in Fig. 18.9(b). In funnel flow, slip occurs within the solid at an angle roughly equal to the angle of internal friction if the solids have low cohesion. In extreme cases, particularly when the solids are cohesive, rat-holes, bridges, or arches can occur (Fig. 18.10). The formation of rat-holes and arches causes numerous problems. Flow is interrupted while the hopper is still largely full, and level detection devices may no longer function correctly. Also, if a bridge or rat-hole in a fine powder collapses suddenly, the void fraction increases rapidly, and uncontrollable flow through the discharge known as *flushing* occurs. Volumetric feeders are neither accurate nor effective if the void fraction of solids varies widely, so hoppers in process service are usually designed to avoid funnel flow.

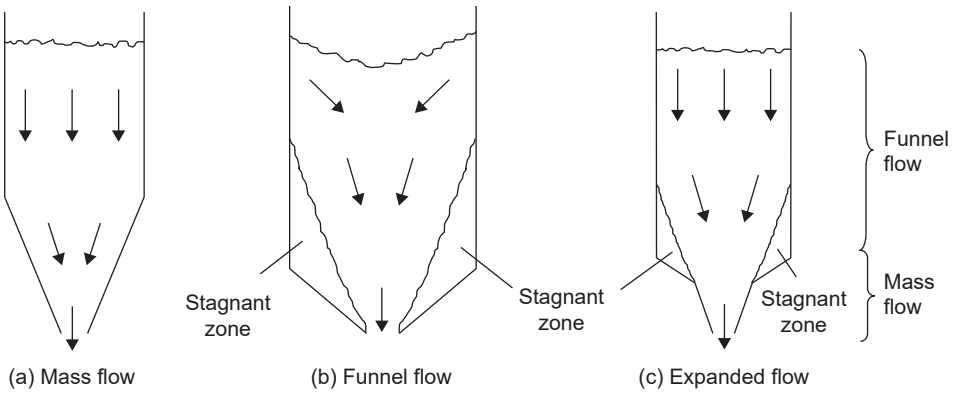


FIG. 18.9 Flow of solid particles from a storage bin.

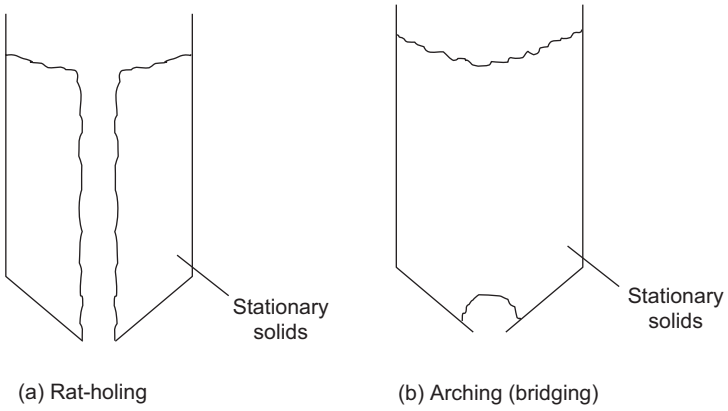


FIG. 18.10 Problems of funnel flow.

One method of avoiding the problems of funnel flow is to use a steep-walled hopper at the base of a funnel flow bin so as to create a mass flow zone at the base with a funnel flow zone above. The entry of the mass flow section is sized to be large enough that a stable arch cannot form. The resulting combination of funnel flow and mass flow is known as expanded flow and is illustrated in Fig. 18.9(c).

Jenike (1967) and Jenike and Johnson (1970) have studied the flow of solids in containers and developed design methods. All aspects of the design of bins and hoppers, including feeding and discharge systems, are covered in books by Reisner (1971) and Brown and Nielsen (1998); see also Rhodes (2008) and the journal articles by Mehos and Maynard (2009), Mehos and Morgan (2016), and Mehos et al. (2018). The use of inserts to correct solids flow problems with existing hoppers is addressed in an article by Bates et al. (2010). The design of large concrete bins and silos is covered by the American Concrete Institute standard ACI-313. See also the British Material Handling Board's code of practice on the design of silos and bunkers: BMHB (1992), Seville et al. (1997), and Thomson (1997). There is no international standard on hopper or silo design at the time of writing.

Flow of solids from an unregulated orifice

The mass flow rate of solids from an open conical hopper or flat-bottomed bin has been shown to be constant and independent of the vessel diameter, D, or depth of solids, H, as long as $H > D$ (Brown & Richards, 1959) and $D > 2.5D_o$, where D_o is the diameter of the opening at the base of the vessel (Fig. 18.11).

Most correlations for solids flow rate are derived from that of Beverloo et al. (1961):

$$m = C\,\rho_b\,g^{1/2}(D_o - k\,d_p)^{5/2} \tag{18.20}$$

where:

m = mass flow rate of solids, kg/s
C = a constant
ρ_b = bulk density, kg/m^3
g = gravitational acceleration, m/s^2
k = a shape parameter
d_p = particle "diameter"

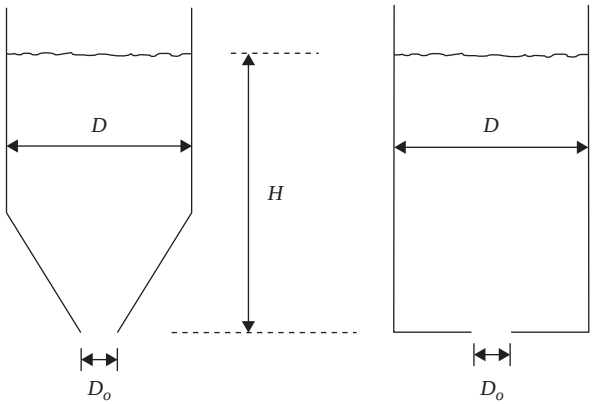


FIG. 18.11 Bin dimensions.

The choice of constant k depends on the measure used for d_p. For uniform spheres, $k = 1.5$, whereas more angular particles have higher values. Beverloo et al. and subsequent workers found quite a large variation in the constant C. It was surmised that this could be because of differences between the bulk density and flowing density of the solids. Nedderman (1992) proposed:

$$m = C' \rho_{bf} g^{1/2} (D_o - k d_p)^{5/2} \tag{18.21}$$

where:

C' = a constant, typically about 0.585
ρ_{bf} = the flowing bulk density of the solids, kg/m^3

The flowing density can be measured at the discharge using γ-ray tomography and is typically 10% to 20% less than the static bulk density (Hosseini-Ashrafi & Tüzün, 1993).

The effects of orifice shape and discharge through side-wall ports are discussed by Dhodapkar et al. (2016).

Note that applying a force to the top of a bed of solids does not improve the flow rate. In fact, conversely, a force on the top of the bed will cause densification of the bed, which increases cohesion and increases the probability of arching or bridging.

Most hoppers are not designed for unregulated flow, as the flow is usually metered into downstream operations. It is, however, important to understand the unregulated flow rate so that the opening is not made too small for the desired design flow rate. To ensure good controllability of the solids flow, the opening is usually sized to allow a much greater flow rate of solids than is needed by the process. The outlet opening must also be large enough to prevent the solids from forming a bridge or arch; see Rhodes (2008).

Volumetric and gravimetric feeders

In most process applications, the flow rate of solids leaving a bin or hopper is governed by a device that ensures a constant flow rate on a volume flow or mass flow basis and that permits the flow to be turned off when necessary. The design of the feeder is an integral part of the design of the bin and hopper. For mass flow to occur in the bin, the feeder shape and opening must allow material to discharge uniformly across the open area at the base of the hopper. The feeder must also allow flow of solids to be interrupted and resumed and must prevent the stationary solids from wicking moisture from downstream fluid operations.

In a *belt feeder* (Fig. 18.12), the base of the hopper section discharges slightly above a conveyor belt. If the belt is stopped, the solids cannot spill out and flow ceases. The volume flow of solids can be varied by adjusting belt speed. Belt feeders are also known as *apron feeders*. A similar principle is used in a *screw feeder* (Fig. 18.13), in which a

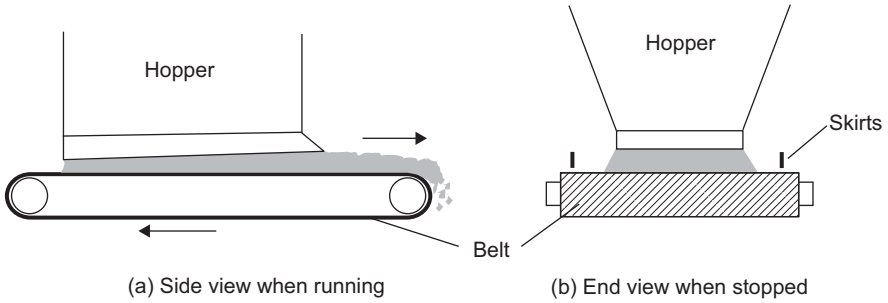


FIG. 18.12 Belt feeder.

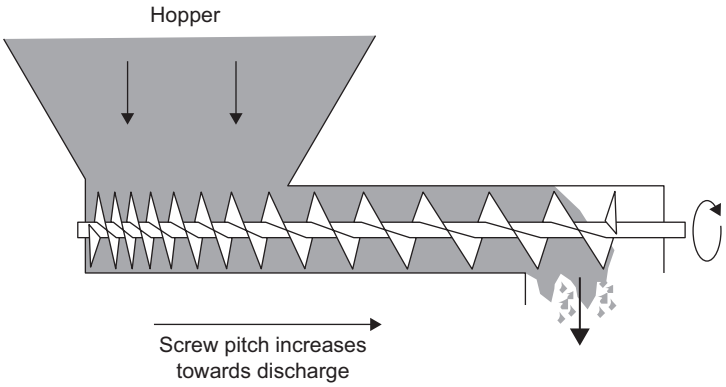


FIG. 18.13 Screw feeder.

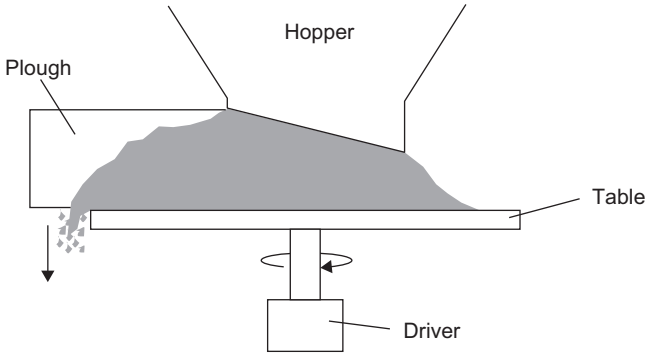


FIG. 18.14 Table feeder.

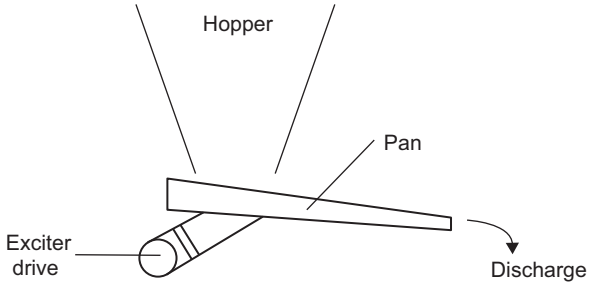


FIG. 18.15 Vibratory feeder.

variable-pitch screw is used to move the solids, and in a *table feeder* (Fig. 18.14), in which the solids discharge onto a rotating table and are scraped off the table by a stationary plow.

For lower solids feed rates that require precise control, a *vibratory feeder*, shown in Fig. 18.15, can be used. With a vibratory feeder, the hopper discharges onto a pan that is vibrated at a controlled speed to give a constant volume flow of solids. Vibratory feeders have a high range of turndown, from 5% to 100% of capacity, but they can be difficult to operate with fine powders that settle or deaerate on the pan.

Rotary feeders (Fig. 18.16) are used for precise control of volume feed rate from larger openings. Rotary feeders are also known as rotary vane feeders or star feeders. The feed rate can be controlled by adjusting the speed of the rotary valve (star valve). The rotary valve can be designed to provide a positive seal between a gas atmosphere in the process and air in the hopper, and the feeder and hopper can be purged with nitrogen if the designer needs to prevent entry of air into the process. Rotary vane feeders are particularly useful when feeding into contained systems such as pneumatic conveyors or fluidized beds. Rotary vane feeders can be prone to jamming when the tolerances between the vanes and casing are small.

Volumetric feeders can only provide a constant mass flow rate to a process if the flowing density of the solids at the hopper discharge remains constant. When more precise control of mass flow rate is needed, a gravimetric feeder must be used. Gravimetric feeders usually consist of a weighing device in line with a volumetric feeder so that the volumetric feeder rate can be adjusted using feedback from the weighing device. Batch and continuous weighing devices are used; see Green and Southard (2018) and Liptak (1993).

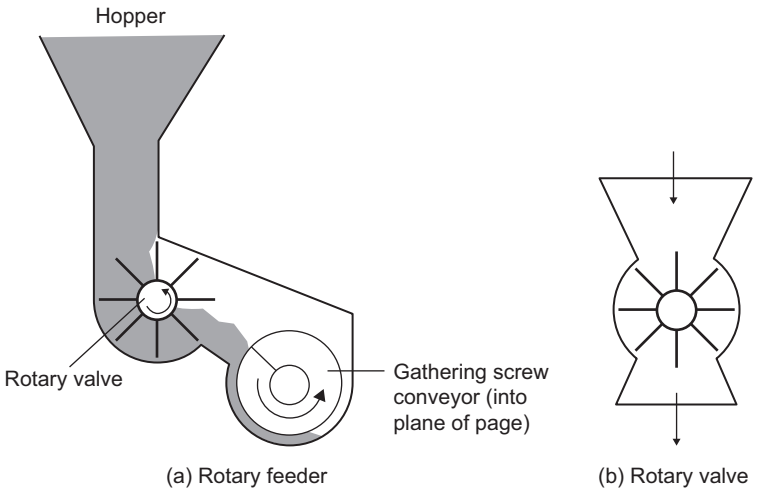


FIG. 18.16 Rotary feeders.

When small bins and hoppers are used, it is sometimes sufficient to place the bin on a load cell and record the loss in mass of the contents against time.

There are many suppliers of bins, hoppers, and feeder systems. Most of them have catalogs or selection tools on their websites that allow preliminary identification of a suitable device for a given application. However, it is always necessary to consult a vendor for a firm warranty that their device is suitable before a final selection is made. It may also be worthwhile to make test runs using the vendor's test facilities, particularly when dealing with cohesive materials or fine powders. Guidelines for feeder selection are given in an article by Marinelli and Miller (2017).

Example 18.1

A tablet-forming process is to be continuously fed with 10 kg/h or USP-grade sorbitol powder when in operation. The sorbitol is supplied in 35-kg polypropylene bags with polyethylene liners, stacked 24 bags to a pallet, minimum order 20 pallets, with 45-day lead time for orders.

Design a storage and feed system for the sorbitol powder. Sorbitol has average bulk density 1.48 kg/liter and can be assumed to have an average particle size of 200 μm.

Solution

Feed rate of 10 kg/h = 240 kg/day, hence 240/35 = 6.9 bags per day, or exactly 2.0 pallets per week.

A minimum order of 20 pallets should therefore last for 10 weeks, which is longer than the 45-day lead time for orders. The plant can therefore order the minimum quantity, placing an order when there are ~14 pallets remaining. This would be sufficient for 49 days operation, thereby allowing 4 days margin above the 45-day delivery lead time quoted.

Because the feed arrives packed in dry bags, there is no need to unpack it immediately. Sufficient warehouse space should be allowed for storage of an incoming order of 20 pallets, plus a few pallets extra to allow for potential interruption of supply. If we allow sufficient storage for an additional 2 weeks of operation (4 pallets), then we would need warehouse space for 24 pallets. A standard pallet is 1.065 × 1.22 m, that is, 1.3 m^2 area, so we need to set aside at least 24 × 1.3 = 31 m^2 of warehouse space, plus allowances for forklift truck movement and access.

The sorbitol must then be transferred from the warehouse to a bin that feeds the process. This will require an operator to move a pallet to the bin twice per week. A suitable elevator, lift, or hoist system must be designed to enable the operators to move the sorbitol bags to the top of the feed bin. In a region with low labor costs, this could be as simple as operators carrying the bags one at a time, although the safety risks of operators carrying 35-kg bags over any significant distance would be deemed unacceptable by most companies. A better design would be to use a hoist or lift to raise the pallet to a platform above the feed bin. Alternatively, a pallet could be loaded into a freight elevator and then the bags could be unloaded manually onto a platform above the feed bin. The hoist can be designed and costed knowing that the mass of the pallet is about 30 kg and the mass of the contents is 24 × 35 = 840 kg, so the hoist should be rated for at least 1000 kg to allow some design margin.

It is not necessary to design the feed bin to hold the entire contents of a pallet of bags, as provision can be made to store a few bags on the platform above the feed bin. In fact, there may be advantages to designing a smaller bin, as it will have a lower residence time and reduce the chance of compaction or moisture adsorption by the sorbitol, which is hygroscopic.

The smallest practical size of feed bin would be sized to hold a single 35-kg bag of feed and would require refilling every $35/10 = 3.5$ hours. This would not be convenient with the usual 8-hour shift cycle, so if we design a feed bin that can hold four bags of sorbitol, then the operators can load two bags at some point during the shift when a low level is indicated by the control system.

$$\text{Bin volume} = \frac{4 \times 35}{1.48} = 95 \text{ liters}$$

Assuming a 2:1 cylindrical bin, volume $= \pi D^3/2$:

$$\text{Bin diameter} = \left(\frac{0.095 \times 2}{\pi}\right)^{1/3} = 0.4 \text{ m}$$

$$\text{Bin height} = 0.8 \text{ m}$$

Using Nedderman's version of the Beverloo equation (Equation 18.21):

$$\frac{10}{3600} = 0.585 \times \left(\frac{1480}{1.2}\right) \times (9.81)^{1/2}\left(D_o - 1.5 \times 200 \times 10^{-6}\right)^{5/2} \tag{18.21}$$

$$D_o = 300 \times 10^{-6} + \left(1.229 \times 10^{-6}\right)^{2/5} = 4.62 \times 10^{-3} \text{ m}$$

A 5-mm opening would obviously be too small for a fine powder such as sorbitol, so a much larger opening would be used in combination with a precise gravimetric feeder. Details of the hopper design and feeder selection can now be worked out in consultation with a vendor. Other factors may also need to be considered, for example, ensuring that the feed system is in accordance with Current Good Manufacturing Practices (CGMP) if the tablet-making process is for food or drug manufacture.

Another alternative that could be considered would be to use a small feeder bin placed at ground level with a screw or pneumatic conveyor to lift the solids into the feed storage bin. The operators would then empty bags into the feeder bin without requiring a hoist or elevator. Several manufacturers supply proprietary designs of such feeder systems. The cost of these proprietary systems could be compared with the cost of the design proposed earlier.

18.3.3 Packaging and storage of solid products

Some solid products such as polymer chips, petroleum coke, and foods such as flour and sugar are shipped in bulk in railroad hopper cars and bulk ship containers. Standard railroad hopper cars in the United States are designed to hold 55 tons or 100 tons. Dimensions of hopper cars are given in Green and Southard (2018).

Most solid products are not suitable for bulk shipment and are packaged in bags or polyethylene-lined 55-gallon drums. A wide variety of bag and drum filling devices exists, and details of specific designs can be obtained from manufacturer's websites. Small sacks are usually designed to be easily lifted by one or two workers and do not hold more than 80 lb (36 kg). Larger sewn bags and flexible containers can hold as much as a metric ton. The filled bags or drums are stacked on standard 1.065 m by 1.22 m pallets and are usually wrapped with stretch-wrap or shrink-wrap or taped to prevent the contents from slipping off the pallet during transportation.

Consumer products, foods, and pharmaceutical products are usually packed directly into the final packaging for quality control purposes and are then boxed for delivery to wholesalers. Because the final packaging contains a relatively small quantity of material (typically less than 1 kg), the packaging operations are highly automated. The food, beverage, and consumer products industries have developed highly integrated systems for weighing (or metering), filling, sealing, inspecting, stacking, and boxing small containers at rates up to the order of ten units per second. Details of packaging and filling equipment must be obtained in consultation with the equipment manufacturer.

18.3.4 Conveying of solids

The movement and storage of solids are usually more expensive than the movement of liquids and gases, which can be easily pumped down a pipeline. The best equipment to use to move solids will depend on a number of factors:

1. The throughput
2. Length of travel

3. Change in elevation
4. Nature of the solids: size, bulk density, angle of repose, angle of wall friction, abrasiveness, corrosiveness, wet or dry

Belt conveyors

Belt conveyors are the most commonly used type of equipment for the continuous transport of solids. They can carry a wide range of materials economically over long and short distances, either horizontally or at an appreciable angle, depending on the angle of repose and angle of wall (belt) friction of the solids. A belt conveyor consists of an endless belt of a flexible material, supported on rollers (idlers), and passing over larger rollers at each end, one of which is driven. The belt material is usually fabric-reinforced rubber or plastic; segmental metal belts are also used. Belts can be specified to withstand abrasive and corrosive materials. The design, installation, operation, and maintenance of conveyor belts are covered in the Conveyor Equipment Manufacturers Association standard (CEMA, 2014) and are also addressed by several international (ISO) standards; see BS EN ISO 21183, BS EN ISO 14890, and BS EN ISO 15236.

Polymer or rubber belt conveyors are restricted to running at ambient conditions and cannot handle hot solids, though metal belts can run hot and are used in belt dryers. The belt width and speed depend on the particle size and bulk density of the material. The lowest cost is obtained by using a narrow belt running at high speed, but dust formation can limit the obtainable speed, particularly if the belt is not covered. Speeds up to 5 ms^{-1} are possible, although 2 to 3 ms^{-1} is most typical. The carrying capacity can be determined from the belt speed, load cross-sectional area, and material bulk density. The load cross-sectional area depends on the angle of repose of the solids, the depth of filling, and whether the conveyor has side idlers to prevent spillage at the sides. Table 18.4, which is adapted from data of Raymus (1984), gives the relationships between belt width, maximum lump size, and load cross-sectional area for a troughed belt with idlers. Load cross-sectional areas for other designs and belt sizes are given in CEMA (2014). Belt conveyors used in mining can be several kilometers long, but most belt conveyors in the process industries are shorter than 100 m.

TABLE 18.4 Belt conveyor capacity

Belt width	Max lump size	Load cross-sectional area			
(in)	(m)	(in)	(mm)	(ft^2)	(m^2)
14	0.35	2.0	51	0.11	0.01
16	0.4	2.5	64	0.14	0.013
20	0.5	3.5	89	0.22	0.02
24	0.6	4.5	114	0.33	0.03
30	0.75	7.0	178	0.53	0.05
36	0.9	8.0	203	0.78	0.072
48	1.2	12.0	305	1.46	0.136
60	1.5	16.0	406	2.40	0.223

Adapted from Raymus (1984).

The power required to operate a belt conveyor is made up of the power required to run the empty belt, the work required to raise or lower the load, and the work required to overcome friction caused by the load moving over the rotating parts and causing flexure or indentation of the belt. The magnitude of each contribution can vary depending on the application (Alspaugh, 2004). For large conveyors carrying high loads of bulk minerals, the power is closely proportional to the mass, as both the potential energy required and the friction at the belt are proportional to the mass conveyed; however, for small conveyors carrying low loads over short distances (as often encountered in the process industries), the power consumption can be a weak function of the mass transported if there is no change in elevation, as the belt itself may make up a significant fraction of the mass moved. Power consumption is therefore best determined in consultation with an equipment vendor. Preliminary estimates of power consumption can be made using process simulation programs that include conveying as a unit operation; see Chapter 4.

The mechanical conveying of solids is the subject of books by Colijn (1985), Fayed and Skocir (1996), Levy and Kalman (2001), and McGlinchey (2008). The conveying of wet solids is addressed by Heywood (1991).

Screw conveyors

Screw conveyors, also called worm conveyors, are used for materials that are free flowing. The basic principle of the screw conveyor has been known since the time of Archimedes. The modern conveyor consists of a helical screw rotating in a U-shaped trough or enclosed pipe. They can be used horizontally or, with some loss of capacity, at an incline to lift materials. Screw conveyors are less efficient than belt conveyors due to the friction between the solids and the flights of the screw and the trough, but are cheaper and easier to maintain. They are used to convey solids over short distances and when some elevation (lift) is required. They can also be used for delivering a metered flow of solids.

Green and Southard (2018) give data on screw conveyor power consumption that can be correlated with the following equation:

$$p = 0.038 + 0.0072 m L_c^{0.8} \tag{18.22}$$

where:

p = power consumption (hp)
m = mass flow (tons/h)
L_c = conveying distance (ft)

Equation 18.22 can be used to obtain a preliminary estimate of the work required for a screw conveyor; however, an accurate estimate will require consultation with a vendor. An excellent overview of screw compressor design is given by Roberts (2015). Screw conveyors are described in detail in the book by Forcade (1999).

Pneumatic and hydraulic conveying

Pneumatic conveying is used for movement of solids over relatively short distances. It is generally suitable only for free-flowing particles in the range of 20 μm to 50 mm, as finer dusts tend to stick to the pipes, while larger particles are hard to entrain. In pneumatic conveying, the solids are transported in suspension in a gas. The solids may be either dilute phase, with void fraction typically greater than 95%, or dense phase, with void fraction as low as 50%. The velocity of carrier fluid must be large enough to keep the particles suspended; see Chhabra and Gurappa (2019). Pneumatic conveying can be used for both horizontal and vertical transport of solids, including making pipe turns. Sharp turns are generally avoided, as these cause solids attrition and pipe abrasion. In a pneumatic conveying system, the solids are usually fed from a hopper via a rotary vane feeder that prevents backflow and are entrained into the gas flow, as shown in Fig. 18.17(b). Pneumatic conveying can also be used under slight vacuum as a means of

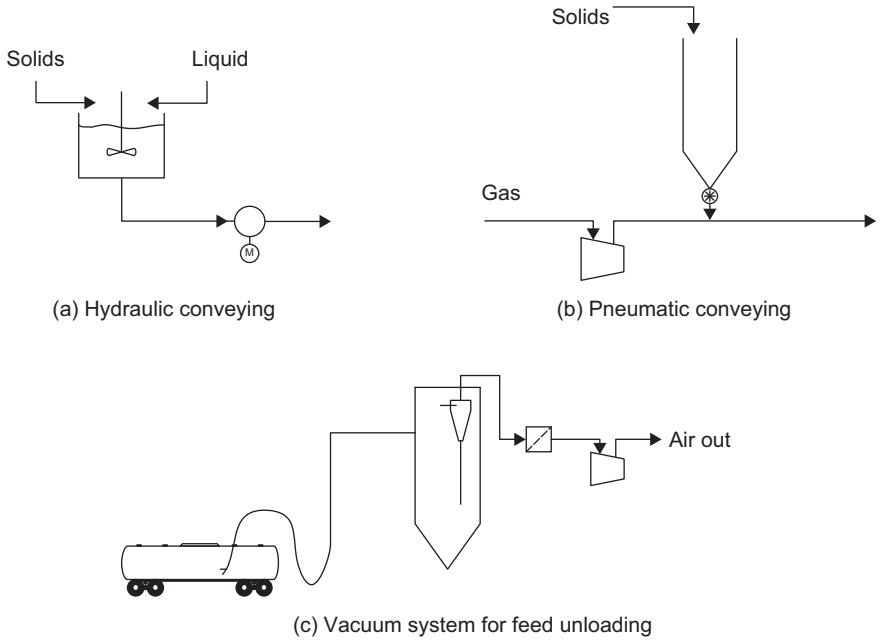


FIG. 18.17 Hydraulic and pneumatic conveying.

unloading feed tankers or lifting solids into silos. A flexible feed hose attached to the silo is used to suck up the solids, rather like a domestic vacuum cleaner. A vacuum compressor is used to pull air out of the silo. A combination of a cyclone and filter will usually be used upstream of the vacuum compressor to prevent damage from particulates, as illustrated in Fig. 18.17(c).

Small, portable pneumatic conveyors with flexible hoses instead of piping are often used for conveying solids over small distances in the manufacture of specialty chemicals and pharmaceuticals.

Hydraulic conveying is similar to pneumatic conveying, but uses a liquid rather than a gas as the carrier fluid. The smaller difference in specific gravity between the particles and carrier fluid makes it easier to entrain solids, but it is much harder to separate the solids from the carrier. Because pumps are less susceptible to damage by solids than compressors, hydraulic conveying systems usually mix the solid and liquid upstream of the pump and then pump the resulting slurry, as shown in Fig. 18.17(a). Hydraulic conveying is widely used in mining, coal processing, and oil drilling, but is only used in the process industries when contamination of the solids with the carrier fluid is acceptable, for example, when processing solids in water or conveying a catalyst in process feed.

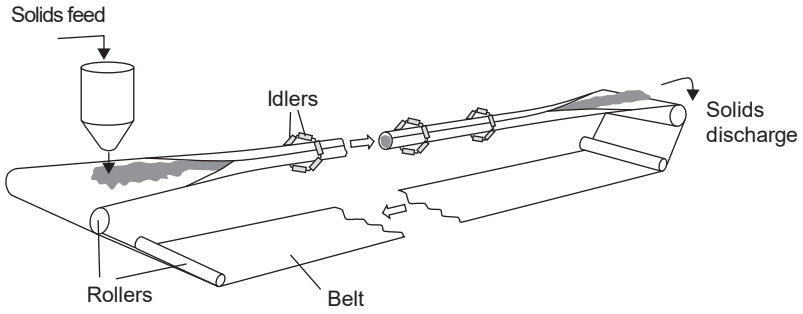
The work required in hydraulic conveying can be estimated from the pipe pressure drop by treating the slurry as a fluid, as described in Section 20.7.2. For pneumatic conveying, the calculation is more complex, as allowance must be made for the compressible nature of the gas and the acceleration that occurs when the solids enter the gas flow. Methods for pressure drop in horizontal and vertical pneumatic conveying are given in Seville et al. (1997) and Jones (1997). Pneumatic and hydraulic conveying are discussed in a book by Mills (2015); see also Mills et al. (2004), Rhodes (2008), and Wilms and Dhodapkar (2014).

Pipe conveyors

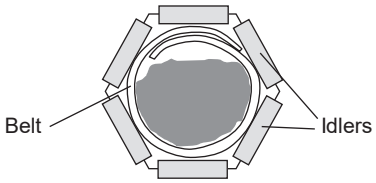
Pipe conveying is a relatively new technology that is becoming widely used in minerals handling. A pipe conveyor is similar to a belt conveyor in that solids are dropped onto a flexible belt. After loading the solids, the belt passes through rollers that fold the sides over to cover the solid (Fig. 18.18). The rolled-up tube containing the solids then passes through idlers that keep the tube rolled until the destination, where the tube is unrolled and the solids are discharged. Pipe conveyors cost only slightly more than belt conveyors and have a number of advantages. They cause less dust formation, there is no need to cover the conveyor to keep material dry, and there is no need for the pipes to follow straight flights, so a pipe conveyor can more easily traverse difficult terrain.

Bucket elevators

The most widely used equipment where a vertical lift is required is the bucket elevator. This consists of buckets fitted to an endless chain or belt, which passes over a driven roller or sprocket at the top end. Bucket elevators can



(a) Overall schematic



(b) Cross-section of "pipe"

FIG. 18.18 Pipe conveyor.

handle a wide range of solids, from heavy lumps to fine powders, and are suitable for use with wet solids and slurries.

18.3.5 Pressurization of solid feeds

Bringing a solid feed into a process that operates under pressure can be challenging, as there will always be a tendency for high-pressure fluids to flow back through the interstitial spaces between solid particles if a positive seal is not provided.

When the process fluid is a nonflammable liquid, the simplest means of pressurizing the solid is to slurry it into the process liquid and then pump the resulting slurry to the desired pressure. This is the same concept as the hydraulic conveying system shown in Fig. 18.17(a). If the process fluid is flammable, it can still be used to slurry the solids, but a closed atmospheric-pressure slurrying tank must be used, and the solids must be fed through a rotary vane feeder or rotary valve that minimizes back-flow of vapor. The head space in the mixing tank should also be vented with inert gas, as shown in Fig. 18.19. Additional treatment of the vent gas may be needed to control particulate (dust) and VOC emissions.

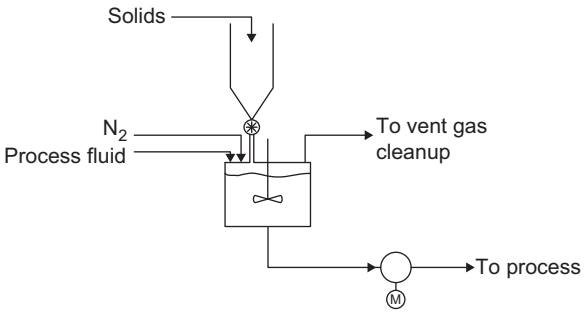


FIG. 18.19 Vented and purged system for feeding solids into hydrocarbon.

For a slurry to be pumpable, the void fraction must be greater than 0.7, and greater than 0.8 is usually preferred. It is therefore necessary to feed roughly four volumes of liquid per volume of solid with this approach. When such high volumes of liquid are unacceptable, a dilute slurry can be prepared, pumped to pressure, and then fed to a hydrocyclone to form a more concentrated slurry. The dilute stream from the hydrocyclone can be recycled to the slurrying tank.

Feeding a solid into a high-pressure gas-phase process is substantially more difficult. Rotary valves and screw conveyors can be designed with tight enough tolerances to prevent gas back-flow for relatively small pressure differences. If the distance between flights on a screw conveyor is tapered, then compression will occur, so a screw conveyor can be designed to act as a solids compressor over a small range of pressure increase.

For larger pressure increases, a *dual hopper* system can be used, as illustrated in Fig. 18.20. Dual hoppers are also known as *charge hoppers* or *lock hoppers*. In a dual hopper arrangement, the solids flow is metered from the upper hopper into the lower hopper while the lower hopper is isolated from the process. The upper hopper is then isolated from the lower hopper and the lower hopper is brought to process pressure, usually by up-flow of gas to avoid compressing the bed of solids. The isolation valve at the lower hopper outlet is then opened to discharge solids into the process. Once the solids are discharged, the lower hopper is isolated, is vented to low pressure, and is

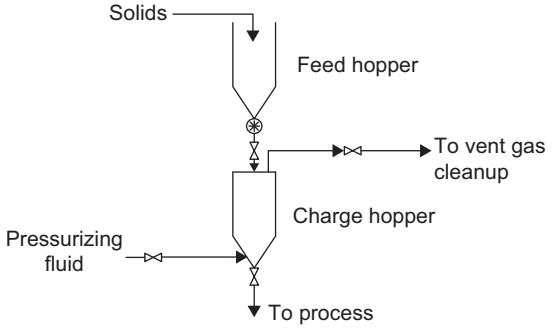


FIG. 18.20 Dual hopper feed system.

then ready to be charged again. The timing of the cycle is set to ensure the desired volumetric or mass flow rate of solids to the process. Specially designed valves are used that can isolate gas flow in the presence of solids. In some designs a double valve arrangement is used, where the upper valve can close on a flowing solids stream, and the lower valve subsequently closes to provide a gas-tight seal.

A dual hopper flow scheme always operates in a semi-batch mode. The design engineer must ensure that the equipment is sized for the actual instantaneous flowing rate of solids or gas and not for the time-averaged flow rate.

Dual hopper schemes can also be used when a solid is moved from an air- or oxygen-containing environment to a hydrogen- or hydrocarbon-containing environment or vice versa. Purging the charge hopper with an inert gas such as steam or nitrogen prevents either flammable gas or oxidant from being entrained with the solids flow.

18.4 Separation and mixing of solids

Processes and equipment are required to separate valuable solids from unwanted material and for size grading (classifying) solid raw materials and products.

The equipment used for solid–solid separation processes was developed primarily for the minerals processing and metallurgical industries for the benefication (upgrading) of ores. The techniques used depend on differences in physical, rather than chemical, properties, though chemical additives may be used to enhance separation. The principal techniques used are shown in Fig. 18.21, which can be used to select the type of processes likely to be suitable for a particular material and size range. Sorting material by appearance, by hand, is now rarely used due to the high cost of labor.

Blending and mixing devices are used when intermingling of particles is desired. Solid particles may require mixing to achieve a desired blend for formulation purposes or to prevent segregation by particle size or density during processing.

18.4.1 Screening (sieving)

Screens separate particles on the basis of size. Their main application is in grading raw materials and products into size ranges, but they are also used for the removal of trash (oversized and undersized contaminants) and for dewatering. Industrial screening equipment is used over a wide range of particle sizes, from fine powders to large rocks. For small particles, woven cloth or wire screens are used, and for larger sizes, perforated metal plates or grids.

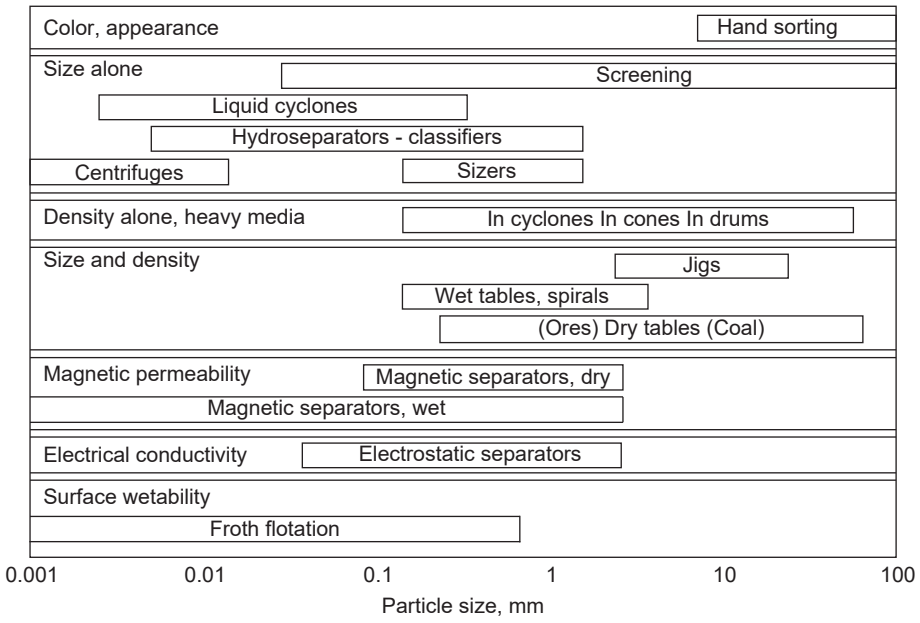


FIG. 18.21 A particle size selection guide to solid–solid separation techniques and equipment. *(From Roberts, E. J., Stavenger, P., Bowersox, J. P., Walton, A. K., & Mehta, M. (1971). Solid/solid separation.* Chemical Engineering, New York, 78*(Feb. 15), 89.)*

Screen sizes are defined in two ways: by a mesh size number for small sizes and by the actual size of opening in the screen for the larger sizes. There are several different standards in use for mesh size, and it is important to quote the particular standard used when specifying particle size ranges by mesh size. In the United States, the appropriate ASTM standards should be used, ASTM E11, but Tyler mesh sizes will often be encountered. For overseas designs the International Organization for Standardization (ISO) standards will usually be used. These are available in English as BS 7792 (ISO 10630) and BS ISO 14315. The relationship between particle size and standard mesh sizes is given in Table 18.1 in Section 18.2.1.

The simplest industrial screening devices are stationary screens, over which the material to be screened flows. Typical of this type are "Grizzly" screens, which consist of rows of equally spaced parallel bars and which are used to "scalp" off oversized rocks in the feed to crushers.

Dynamic screening equipment can be categorized according to the type of motion used to shake up and transport the material on the screen. The principal types used in the chemical process industries are described briefly next.

Vibrating screens: Horizontal and inclined screening surfaces vibrated at high frequencies (1000 to 7000 Hz). These are high-capacity units, with good separating efficiency, and are used for a wide range of particle sizes.
Oscillating screens: Operated at lower frequencies than vibrating screens (100 to 400 Hz) with a longer, more linear stroke.
Reciprocating screens: Operated with a shaking motion, a long stroke at low frequency (20 to 200 Hz). Used for conveying with size separation.
Sifting screens: Operated with a circular motion in the plane of the screening surface. The actual motion may be circular, gyratory, or circularly vibrated. Used for the wet and dry screening of fine powders.
Revolving screens: Inclined, cylindrical screens rotated at low speeds (10 to 20 rpm). Used for the wet screening of relatively coarse material, but have now been largely replaced by vibrating screens.

Fig. 18.22, which is based on a similar chart given by Matthews (1971), can be used to select the type of screening equipment likely to be suitable for a particular size range. Equipment selection will normally be based on laboratory and pilot-scale screening tests conducted by the equipment vendors or with their cooperation. The main factors to be considered, and the information that would be required by the firms supplying proprietary screening equipment, are listed here:

1. Rate, throughput required
2. Size range (test screen analysis)
3. Characteristics of the material: free-flowing or sticky, bulk density, abrasiveness
4. Hazards: flammability, toxicity, dust explosion
5. Wet or dry screening to be used

18.4.2 Liquid–solid cyclones

Cyclones can be used for the classification of solids, as well as for liquid–solid and liquid–liquid separations. The design and application of liquid cyclones (hydrocyclones) is discussed in Section 18.6.4. A typical unit is shown in Fig. 18.23.

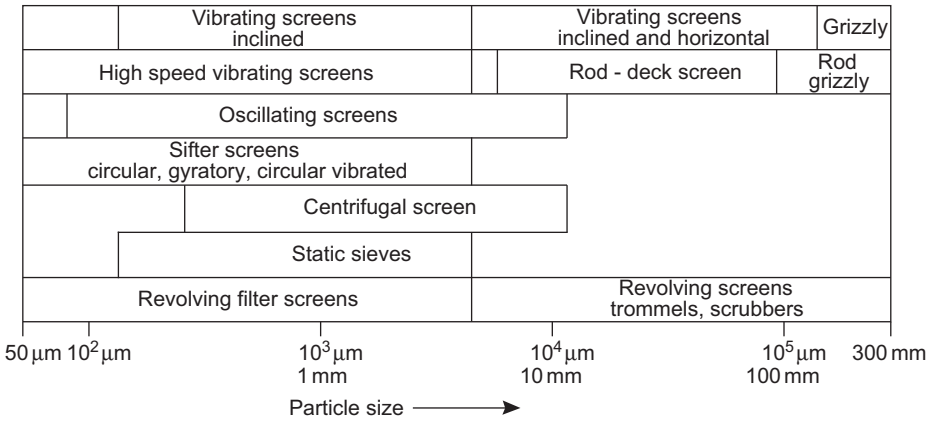


FIG. 18.22 Screen selection by particle size range.

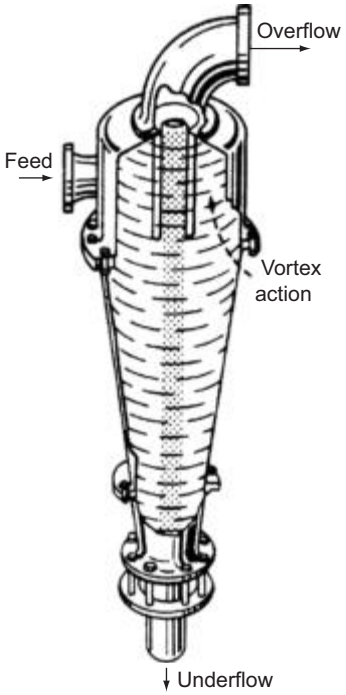


FIG. 18.23 Liquid–solid cyclone (hydrocyclone).

Liquid cyclones can be used for the classification of solid particles over a size range from 5 to 100 μm. Commercial units are available in a wide range of materials of construction and sizes, from as small as 10 mm to up to 30 m in diameter. The separating efficiency of liquid cyclones depends on the particle size and density and the density and viscosity of the liquid medium.

18.4.3 Hydroseparators and sizers (classifiers)

Classifiers that depend on the difference in the settling rates of different size particles in water are frequently used for separating fine particles in the 50 to 300 μm range. Various designs are used. The principal ones used in the chemical process industries are described next.

Thickeners: Thickeners are primarily used for liquid–solid separation (see Section 18.6). When used for classification, the feed rate is such that the overflow rate is greater than the settling rate of the slurry, and the finer particles remain in the overflow stream.

Rake classifiers: These are inclined, shallow, rectangular troughs fitted with mechanical rakes at the bottom to rake the deposited solids to the top of the incline (Fig. 18.24). Several rake classifiers can be used in series to separate the feed into different size ranges.

Bowl classifiers: These are shallow bowls with concave bottoms fitted with rakes. Their operation is similar to that of thickeners.

18.4.4 Hydraulic jigs

Jigs separate solids by difference in density and size. The material is immersed in water, supported on a screen (Fig. 18.25). Pulses of water are forced through the bed of material either by moving the screen or by pulsating the water level. The flow of water fluidizes the bed and causes the solids to stratify with the lighter material at the top and the heavier at the bottom.

18.4.5 Tables

Tables are used wet and dry. The separating action of a wet table resembles that of the traditional miner's pan. Riffled tables (Fig. 18.26) are basically rectangular decks, inclined at a shallow angle to the horizontal (2 to 5 degrees),

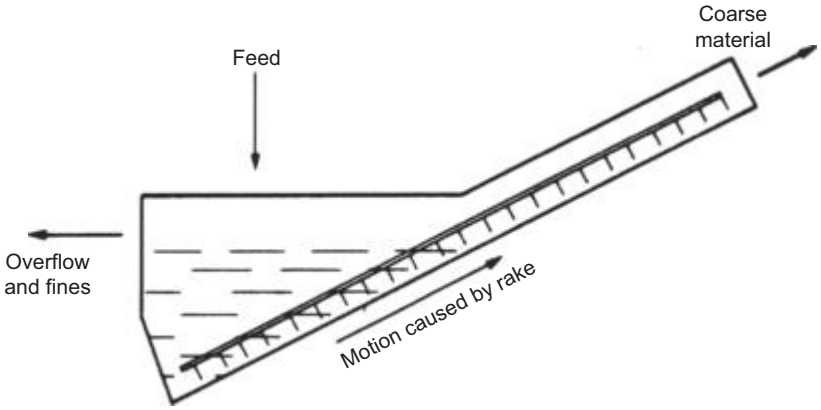


FIG. 18.24 Rake classifier.

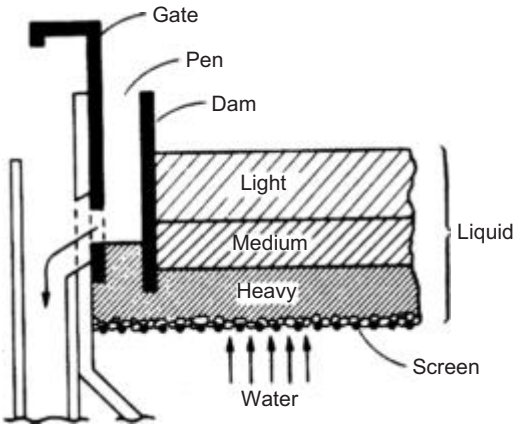


FIG. 18.25 A hydraulic jig.

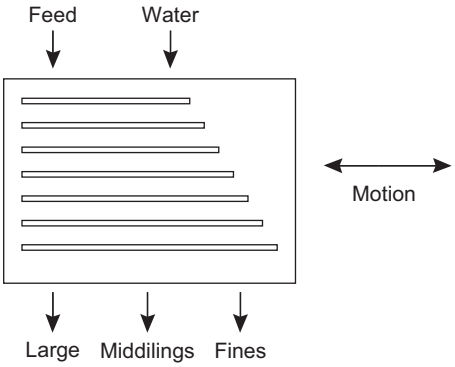


FIG. 18.26 Wilfley riffled table.

with shallow slats (riffles) fitted to the surface. The table is mechanically shaken, with a slow stroke in the forward direction and a faster backward stroke. The particles are separated into different size ranges under the combined action of the vibration, water flow, and resistance to flow over the riffles.

18.4.6 Classifying centrifuges

Centrifuges are used for the classification of particles in size ranges below 10 μm. Two types are used: solid bowl centrifuges, usually with a cylindrical, conical bowl, rotated about a horizontal axis and "nozzle" bowl machines, fitted with discs. These types are described in Section 18.6.3.

18.4.7 Dense-medium separators (sink and float processes)

Solids of different densities can be separated by immersing them in a fluid of intermediate density. The heavier solids sink to the bottom and the lighter float to the surface. Water suspensions of fine particles are often used as the dense liquid (heavy-medium). The technique is widely used in the benefication (concentration) of mineral ores.

18.4.8 Flotation separators (froth-flotation)

Froth-flotation processes are used extensively for the separation of finely divided solids. Separation depends on differences in the surface properties of the materials. The particles are suspended in an aerated liquid (usually water), and air bubbles adhere preferentially to the particles of one component and bring them to the surface. Frothing agents are used so that the separated material is held on the surface as froth and can be removed.

Froth-flotation is an extensively used separation technique, having a wide range of applications in the minerals processing industries and other industries. It can be used for particles in the size range from 50 to 400 μm.

18.4.9 Magnetic separators

Magnetic separators can be used for materials that are affected by magnetic fields; the principle is illustrated in Fig. 18.27. Rotating-drum magnetic separators are used in the minerals processing industries. They can be designed to handle relatively high throughputs, up to 3000 kg/h per meter length of drum. Simple magnetic separators are often used for the removal of iron from the feed to a crusher.

The various types of magnetic separators used and their applications are described by Bronkala (1988).

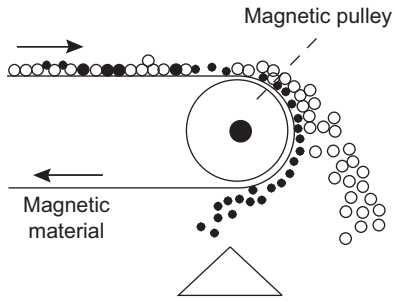


FIG. 18.27 Magnetic separator.

18.4.10 Electrostatic separators

Electrostatic separation depends on differences in the electrical properties (conductivity) of the materials to be treated. In a typical process the particles pass through a high-voltage electric field as they are fed on to a revolving drum, which is at earth potential (Fig. 18.28). Those particles that acquire a charge adhere to the drum surface and are carried further around the drum before being discharged.

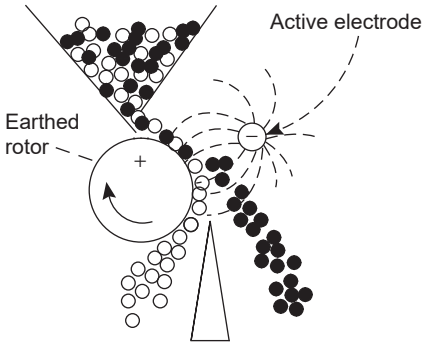


FIG. 18.28 Electrostatic separator.

18.4.11 Solids blending and mixing

Many solid products are blends of different solid materials. Familiar examples include food mixes, soap powders, candy mixes, and lawn fertilizer. Much of the equipment used for mixing solid powders and blending solids into liquids was initially developed for use in the food processing industry. Blends of powders or particulates are also used in the preparation of formed solids such as tablets, catalyst pellets, and many polymer products. Some processes also require solids mixing to prevent segregation of particles by size during processing.

Mixing of solids can be accomplished with or without changes in size distribution. Substantial mixing occurs in size reduction devices; see Section 18.9.

A great variety of specialized equipment has been developed for mixing dry solids and pastes (wet solids). The principal types of equipment and their fields of application are given in Table 18.5. Descriptions of the equipment can be found in the literature: Green and Southard (2018), Harnby et al. (1997), and Reid (1979). A selection chart for solids mixing equipment is given by Jones (1985).

Most solids mixing devices are operated in batch mode. A charge of solids is loaded into the mixer, which is then run for the desired time to achieve mixing and unloaded. Cone blenders are used for free-flowing solids. Ribbon blenders can be used for dry solids and for blending liquids with solids. Z-blade mixers and pan mixers are used for kneading heavy pastes and doughs. Ribbon blenders, fluidized mixers, and paddle mixers can be operated in continuous mode. Static mixers are always operated continuously in a flowing fluid. The power requirement for mixing solids depends on the device used and should be determined in consultation with the device manufacturer or through plant trials. Most manufacturers state the power consumption in their brochures or on their websites. More information on solids mixing is given in Weinekötter and Gericke (2000), Kaye (1996), Green and Southard (2018), Fayed and Otten (1997), and Paul et al. (2003).

TABLE 18.5 Solids and paste mixers

Type of equipment	Mixing action	Applications	Examples
Rotating: cone, double cone, drum	Tumbling action	Blending dry, free-flowing powders, granules, crystals	Pharmaceuticals, food, chemicals
Air blast fluidization	Air blast lifts and mixes particles	Dry powders and granules	Milk powder; detergents, chemicals
Horizontal trough mixer, with ribbon blades, paddles, or beaters	Rotating element produces contra-flow movement of materials	Dry and moist powders	Chemicals, food, pigments, tablet granulation
Z-blade mixers	Shearing and kneading by the specially shaped blades	Mixing heavy pastes, creams, and doughs	Bakery industry, rubber doughs, plastic dispersions
Pan mixers	Vertical, rotating paddles, often with planetary motion	Mixing, whipping, and kneading of materials ranging from low-viscosity pastes to stiff doughs	Food, pharmaceuticals and chemicals, printing inks, and ceramics
Cylinder mixers, single and double	Shearing and kneading action	Compounding of rubbers and plastics	Rubbers, plastics, and pigment dispersion

Tumbling drums

The simplest solids mixers are rotating drums known as tumblers. These are usually double-cone shaped, as shown in Fig. 18.29(a), but twin-shell, V-shaped drums are also used. Tumblers can contain baffles or internals to break up agglomerates and promote mixing. They are generally operated at low speed and are suitable for gentle blending without changes in particle size distribution.

Internally agitated mixers

Several mixer designs use a static drum with moving internals to accomplish mixing of the solids. In a ribbon blender, illustrated schematically in Fig. 18.29(b), a helical ribbon rotates horizontally inside a drum to blend the solids. Vertical screw mixers, shown in Fig. 18.29(c), also use a screw, which lifts the solids along the wall of the vessel and orbits around a central axis. This type is often referred to as a Nauta mixer. In a paddle mixer (see Fig. 18.29d), a horizontal drum containing the solids is agitated by pins or paddles located along a central shaft. Twin-screw paddle mixers are also used, in which two shafts are located in the drum or tank.

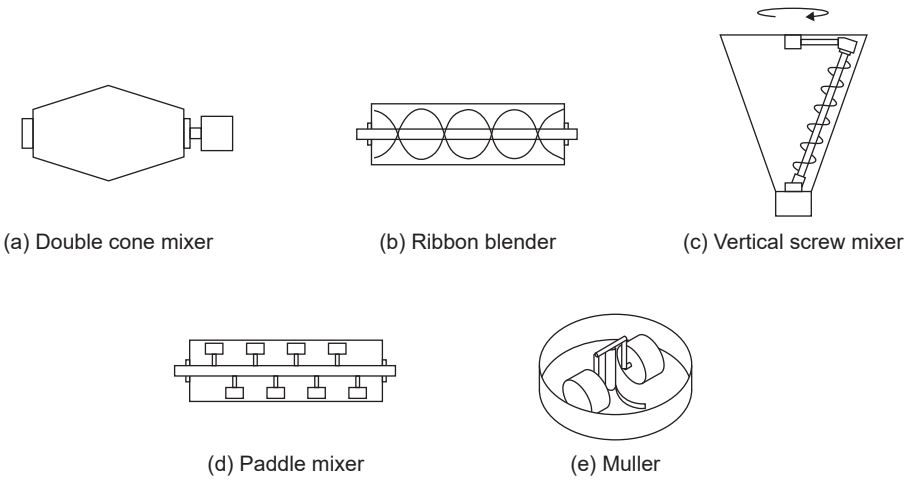


FIG. 18.29 Solids mixers.

A muller, illustrated in Fig. 18.29(e), is an open-pan mixer in which heavy rollers are driven over the material. A plow or scrapers is also incorporated to lift and turn the solids. In some mullers the pans also rotate in the opposite direction to the rollers. Mullers are suitable for materials that agglomerate but are not sticky.

Fluidized mixers

A fluidized bed can be operated to give rapid mixing of solid particles. Fluidized bed mixers can be operated continuously or in batch mode. The mixed particles can be removed continuously from the bed through a stand pipe during operation. Fluidization is discussed in more detail in Section 18.2.2. Fluidized mixers are easily integrated with pneumatic or hydraulic conveying systems.

Static mixers

Static mixers, also known as in-line mixers, can be used to prevent settling of particles or segregation of particles by size during pneumatic or hydraulic conveying. Several different proprietary designs are used, all based on the principle of using shaped internals to break up the flow pattern and remix the solid particles. Static mixers are also used for mixing liquid streams; a typical design is illustrated in Fig. 15.10.

18.5 Gas–solids separations (gas cleaning)

The primary need for gas–solid separation processes is for gas cleaning: the removal of dispersed, finely divided solids (dust) and liquid mists from gas streams. Process gas streams must often be cleaned up to prevent contamination of catalysts or products and to avoid damage to equipment, such as compressors. Also, effluent gas streams must be cleaned to comply with air pollution regulations and for reasons of hygiene, to remove toxic and other hazardous materials; see Muir (1992) and Section 11.5.1.

There is often a need for clean, filtered air for processes that use air as a raw material and where clean working atmospheres are needed: for instance, in the pharmaceutical and electronics industries. Air for process instruments must be clean, dry, and dust-free.

The particles to be removed may range in size from large molecules, measuring a few hundredths of a micrometer, to the coarse dusts arising from the attrition of catalysts or fly ash from the combustion of pulverized fuels.

A variety of equipment has been developed for gas cleaning. The principal types used in the process industries are listed in Table 18.6, which is adapted from a selection guide given by Sargent (1971). Table 18.6 shows the general field of application of each type in terms of the particle size separated, the expected separation efficiency, and the throughput. It can be used to make a preliminary selection of the type of equipment likely to be suitable for a particular application. Descriptions of the equipment shown in Table 18.6 can be found in various handbooks: Green and Southard (2018) and Schweitzer (1997) and in specialist texts: Strauss (1975). Gas cleaning is also covered in Chhabra and Gurappa (2019).

TABLE 18.6 Gas-cleaning equipment

Type of equipment	Minimum particle size (μm)	Minimum loading (mg/m^3)	Approx. efficiency (%)	Typical gas velocity (m/s)	Maximum capacity (m^3/s)	Gas pressure drop (mm H_2O)	Liquid rate ($m^3/10^3$ m^3 gas)	Space required (relative)
Dry collectors								
Settling chamber	50	12,000	50	1.5–3	none	5	—	Large
Baffle chamber	50	12,000	50	5–10	none	3–12	—	Medium
Louver	20	2500	80	10–20	15	10–50	—	Small
Cyclone	10	2500	85	10–20	25	10–70	—	Medium
Multiple cyclone	5	2500	95	10–20	100	50–150	—	Small
Impingement	10	2500	90	15–30	none	25–50	—	Small
Wet scrubbers								
Gravity spray	10	2500	70	0.5–1	50	25	0.05–0.3	Medium
Centrifugal	5	2500	90	10–20	50	50–150	0.1–1.0	Medium
Impingement	5	2500	95	15–30	50	50–200	0.1–0.7	Medium
Packed	5	250	90	0.5–1	25	25–250	0.7–2.0	Medium
Jet	0.5 to 5 (range)	250	90	10–100	50	none	7–14	Small
Venturi	0.5	250	99	50–200	50	250–750	0.4–1.4	Small
Others								
Fabric filters	0.2	250	99	0.01–0.1	100	50–150	—	Large
Electrostatic								
Precipitators	2	250	99	5–30	1000	5–25	—	Large

Gas-cleaning equipment can be classified according to the mechanism employed to separate the particles: gravity settling, impingement, centrifugal force, filtering, washing, and electrostatic precipitation.

18.5.1 Gravity settlers (settling chambers)

Settling chambers are the simplest form of industrial gas-cleaning equipment but have only a limited use; they are suitable for coarse dusts, particles larger than 50 μm. They are essentially long, horizontal, rectangular chambers through which the gas flows. The solids settle under gravity and are removed from the bottom of the chamber. Horizontal plates or vertical baffles are used in some designs to improve the separation. Settling chambers offer little resistance to the gas flow and can be designed for operation at high temperature and high pressure and for use in corrosive atmospheres.

The length of chamber required to settle a given particle size can be estimated from the settling velocity (calculated using Stokes law) and the gas velocity. A design procedure is given by Jacob and Dhodapkar (1997).

18.5.2 Impingement separators

Impingement separators employ baffles to achieve the separation. The gas stream flows easily around the baffles, whereas the solid particles, due to their higher momentum, tend to continue in their line of flight, strike the baffles, and are collected. Many different baffle designs are used in commercial equipment; a typical example is shown in Fig. 18.30. Impingement separators cause a higher pressure drop than settling chambers but are capable of separating smaller particle sizes: 10 to 20 μm.

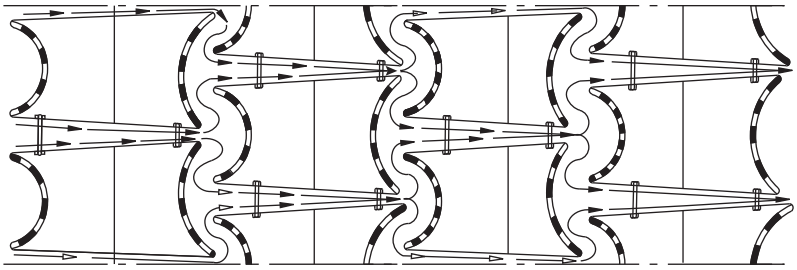


FIG. 18.30 Impingement separator (section showing gas flow).

18.5.3 Centrifugal separators (cyclones)

Cyclones are the principal type of gas–solids separator employing centrifugal force and are widely used. They are simple constructions, can be made from a wide range of materials, and can be designed for high-temperature and high-pressure operation.

Cyclones are suitable for separating particles above about 5 μm in diameter; smaller particles, down to about 0.5 μm, can be separated when agglomeration occurs.

The most commonly used design is the reverse-flow cyclone (Fig. 18.31); other configurations are used for special purposes. In a reverse-flow cyclone the gas enters the top chamber tangentially and spirals down to the apex of the conical section; it then moves upward in a second smaller-diameter spiral and exits at the top through a central vertical pipe. The solids move radially to the walls, slide down the walls, and are collected at the bottom. Design procedures for cyclones are given by Constantinescu (1984). Strauss (1975), Koch and Licht (1977), and Stairmand (1951). The theoretical concepts and experimental work on which the design methods are based are discussed in Chhabra and Gurappa (2019). Stairmand's method is outlined here and illustrated in Example 18.2.

Cyclone design

Stairmand developed two standard designs for gas–solid cyclones: a high-efficiency cyclone (Fig. 18.32a) and a high-throughput design (Fig. 18.32b). The performance curves for these designs, obtained experimentally under standard test conditions, are shown in Figs 18.33(a) and 18.33(b). These curves can be transformed to other cyclone sizes and operating conditions by use of the following scaling equation for a given separating efficiency:

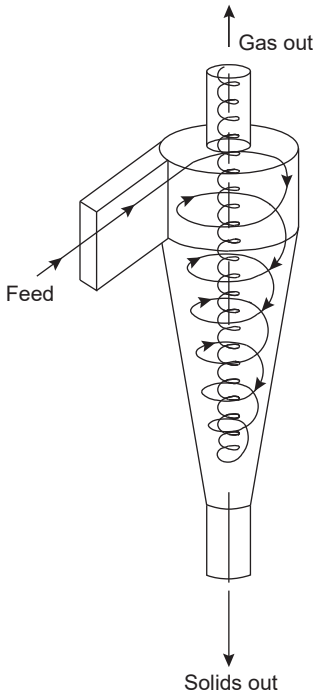


FIG. 18.31 Reverse-flow cyclone.

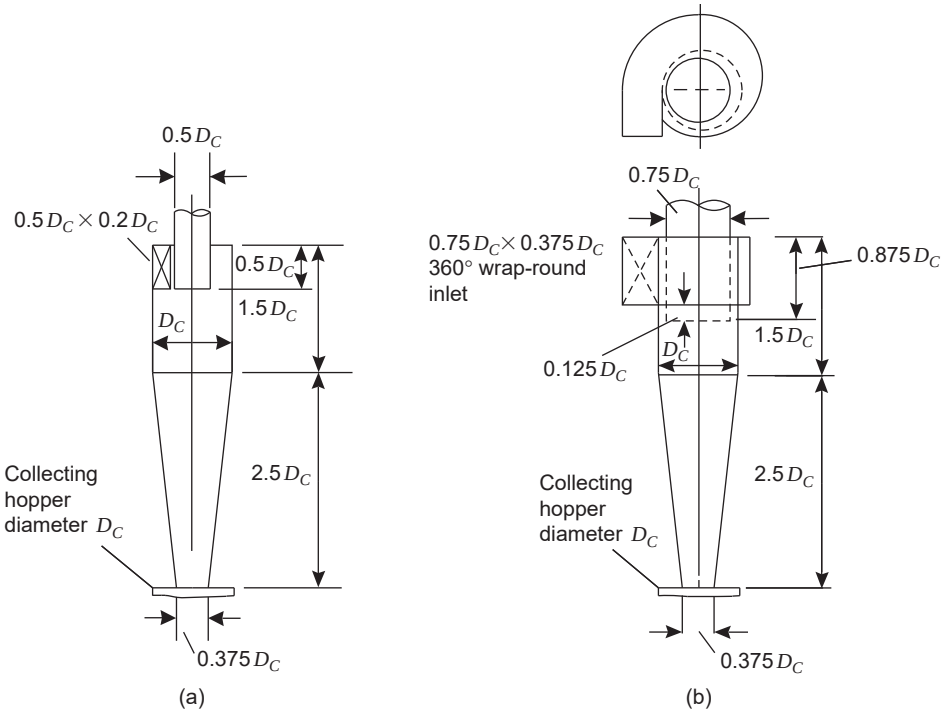
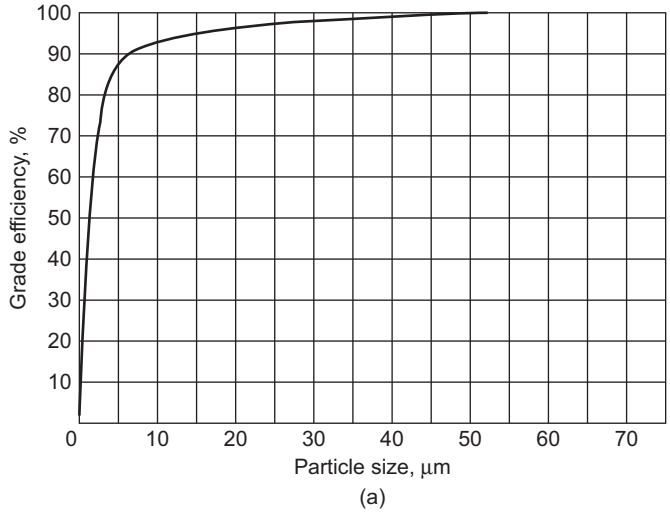


FIG. 18.32 Standard cyclone dimension. (a) High-efficiency cyclone. (b) High-gas-rate cyclone.



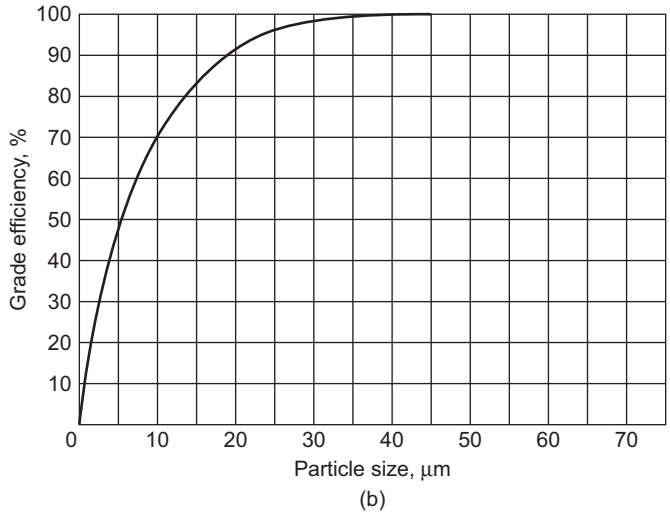


FIG. 18.33 Performance curves, standard conditions. (a) High-efficiency cyclone performance curves, standard conditions. (b) High-gas-rate cyclone.

$$d_2 = d_1 \left[\left(\frac{D_{c_2}}{D_{c_1}} \right)^3 \times \frac{Q_1}{Q_2} \times \frac{\Delta\rho_1}{\Delta\rho_2} \times \frac{\mu_2}{\mu_1} \right]^{1/2} \tag{18.23}$$

where d_1 = mean diameter of particle separated at the standard conditions, at the chosen separating efficiency (see Figs. 18.33a or 18.33b)
d_2 = mean diameter of the particle separated in the proposed design at the same separating efficiency
D_{c_1} = diameter of the standard cyclone = 8 in (203 mm)
D_{c_2} = diameter of proposed cyclone, mm
Q_1 = standard flow rate:
for high efficiency design = 223 m^3/h
for high throughput design = 669 m^3/h
Q_2 = proposed flow rate, m^3/h
$\Delta\rho_1$ = solid–fluid density difference in standard conditions = 2000 kg/m^3
$\Delta\rho_2$ = density difference, proposed design
μ_1 = test fluid viscosity (air at 1 atm, 20 °C) = 0.018 mN s/m^2
μ_2 = viscosity, proposed fluid

A performance curve for the proposed design can be drawn up from Fig. 18.33(a) or 18.33(b) by multiplying the grade diameter at, say, each 10% increment of efficiency by the scaling factor given by Equation 18.23, as shown in Fig. 18.34.

An alternative method of using the scaling factor that does not require redrawing the performance curve is used in Example 18.2. The cyclone should be designed to give an inlet velocity of between 9 and 27 m/s (30 to 90 ft/s); the optimum inlet velocity has been found to be 15 m/s (50 ft/s).

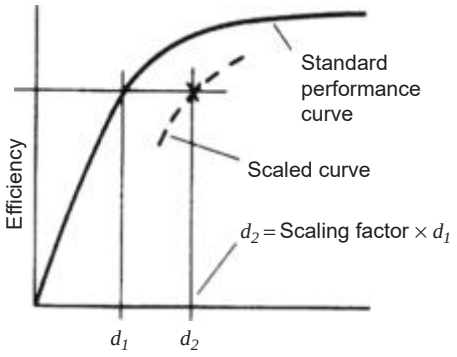


FIG. 18.34 Scaled performance curve.

Pressure drop

The pressure drop in a cyclone will be due to the entry and exit losses and friction and kinetic energy losses in the cyclone. The empirical equation given by Stairmand (1949) can be used to estimate the pressure drop:

$$\Delta P = \frac{\rho_f}{203}\left\{u_1^2\left[1+2\phi^2\left(\frac{2r_t}{r_e}-1\right)\right]+2u_2^2\right\} \tag{18.24}$$

where ΔP = cyclone pressure drop, millibars
ρ_f = fluid (gas) density, kg/m^3
u_1 = inlet duct velocity, m/s
u_2 = exit duct velocity, m/s
r_t = radius of circle to which the center line of the inlet is tangential, m
r_e = radius of exit pipe, m
ϕ = factor from Fig. 18.35
Ψ = parameter in Fig. 18.35, given by:

$$\Psi = f_c\frac{A_s}{A_1}$$

f_c = friction factor, taken as 0.005 for gases
A_s = surface area of cyclone exposed to the spinning fluid, m^2
For design purposes, this can be taken as equal to the surface area of a cylinder with the same diameter as the cyclone and length equal to the total height of the cyclone (barrel plus cone).
A_1 = area of inlet duct, m^2

Stairmand's equation is for the gas flowing alone, containing no solids. The presence of solids will normally increase the pressure drop over that calculated using Equation 18.24, depending on the solids loading. Alternative design methods for cyclones, which include procedures for estimating the true pressure drop, are given by Green and Southard (2018) and Yang (1999); see also Zenz (2001).

General design procedure

1. Select either the high-efficiency or high-throughput design, depending on the performance required.
2. Obtain an estimate of the particle size distribution of the solids in the stream to be treated.
3. Estimate the number of cyclones needed in parallel.

4. Calculate the cyclone diameter for an inlet velocity of 15 m/s (50 ft/s). Scale the other cyclone dimensions from Fig. 18.32(a) or 18.32(b).
5. Calculate the scale-up factor for the transposition of Fig. 18.33(a) or 18.33(b).
6. Calculate the cyclone performance and overall efficiency (recovery of solids). If unsatisfactory, try a smaller diameter.
7. Calculate the cyclone pressure drop and, if required, select a suitable blower.
8. Cost the system and optimize to make the best use of the pressure drop available or, if a blower is required, to give the lowest operating cost.

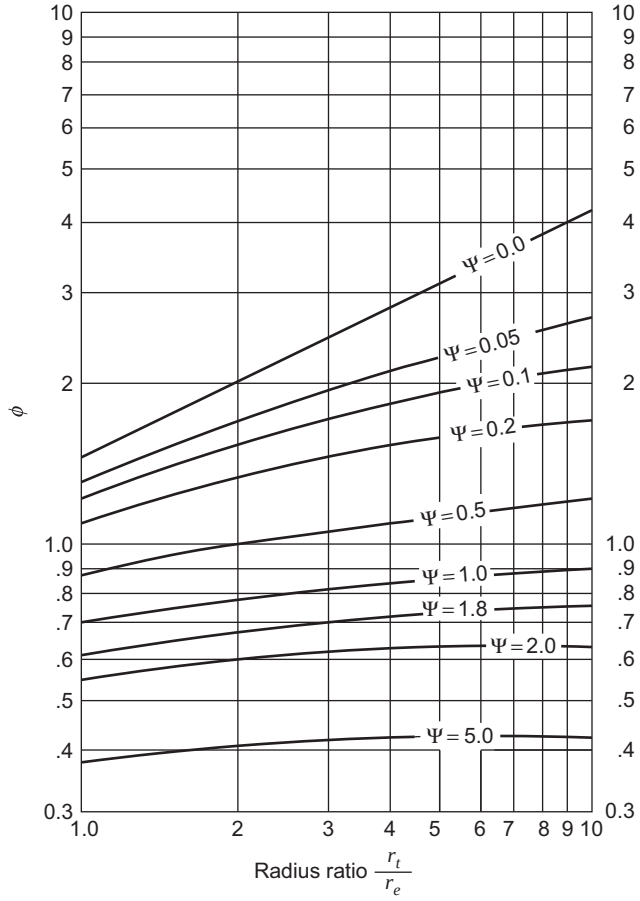


FIG. 18.35 Cyclone pressure drop factor.

Example 18.2

Design a cyclone to recover solids from a process gas stream. The anticipated particle size distribution in the inlet gas is given here. The density of the particles is 2500 kg/m^3, and the gas is essentially nitrogen at 150 °C. The stream volumetric flow rate is 4000 m^3/h, and the operation is at atmospheric pressure. An 80% recovery of the solids is required.

Particle size, μm	50	40	30	20	10	5	2
Percentage by weight less than	90	75	65	55	30	10	4

Solution

As 30% of the particles are below 10 μm, the high-efficiency design will be required to give the specified recovery.

$$\text{Flow rate} = \frac{4000}{3600} = 1.11 \text{ m}^3/\text{s}$$

$$\text{Area of inlet duct, at 15 m/s} = \frac{1.11}{15} = 0.07 \text{ m}^2$$

From Fig. 18.32(a), duct area $= 0.5\ D_c \times 0.2\ D_c$,

$$\text{so, } D_c = 0.84 \text{ m}$$

This is clearly too large compared with the standard design diameter of 0.203 m.
Try four cyclones in parallel, $D_c = 0.42$ m.

$$\text{Flow rate per cyclone} = 1000 \text{ m}^3/\text{h}$$

$$\text{Density of gas at 150 °C} = \frac{28}{22.4} \times \frac{273}{423} = 0.81 \text{ kg/m}^2,$$

This is negligible compared with the solids density:

$$\text{Viscosity of } N_2 \text{ at 150 °C} = 0.023 \text{ cp(mN s/m)}$$

From Equation 18.23,

$$\text{scaling factor} = \left[\left(\frac{0.42}{0.203}\right)^3 \times \frac{223}{1000} \times \frac{2000}{2500} \times \frac{0.023}{0.018}\right]^{1/2} = \underline{\underline{1.42}}$$

The performance calculations, using this scaling factor and Fig. 18.33(a), are set out in the following table:

Calculated performance of cyclone design, Example 18.2

1 Particle size (μm)	2 Percent in range	3 Mean particle size ÷ scaling	4 Efficiency at scaled size % Factor	5 Collected $\frac{(2)\times(4)}{100}$ (Fig. 18.33a)	6 Grading at exit (2) − (5)	7 Percent at exit
>50	10	35	98	9.8	0.2	1.8
50–40	15	32	97	14.6	0.4	3.5
40–30	10	25	96	9.6	0.4	3.5
30–20	10	18	95	9.5	0.5	4.4
20–10	25	11	93	23.3	1.7	15.1
10–5	20	5	86	17.2	2.8	24.8
5–2	6	3	72	4.3	1.7	15.1
2–0	4	1	10	0.4	3.6	31.8
		100	Overall collection Efficiency	88.7	11.3	100.0

The collection efficiencies shown in column 4 of the table were read from Fig. 18.33(a) at the scaled particle size, column 3. The overall collection efficiency satisfies the specified solids recovery. The proposed design with dimensions in the proportions given in Fig. 18.32(a) is shown in Fig. 18.36.

Pressure-drop calculation

$$\text{Area of inlet duct, } A_1, = 210 \times 80 = 16,800 \text{ mm}^2$$

$$\text{Cyclone surface area, } A_s = \pi \times 420 \times (630 + 1050)$$

$$= 2.218 \times 10^6 \text{ mm}^2$$

f_c taken as 0.005:

$$\Psi = \frac{f_c, A_s}{A_1} = \frac{0.005 \times 2.218 \times 10^6}{16,800} = 0.66$$

$$\frac{r_t}{r_e} = \frac{(420 - (80/2))}{210} = 1.81$$

From Fig. 18.35, $\phi = 0.9$.

$$u_1 = \frac{1000}{3600} \times \frac{10^6}{16,800} = 16.5 \text{ m/s}$$

$$\text{Area of exit pipe } = \frac{\pi \times 210^2}{4} = 34,636 \text{ mm}^2$$

$$u_2 = \frac{1000}{3600} \times \frac{10^6}{34,636} = 8.0 \text{ m/s}$$

From Equation 18.24:

$$\Delta P = \frac{0.81}{203}\left[16.5^2\left[1 + 2 \times 0.9^2(2 \times 1.81 - 1)\right] + 2 \times 8.0^2\right]$$

$$= \underline{\underline{6.4 \text{ millibar}}} \text{ (67 mm H2O)}$$

This pressure drop looks reasonable.

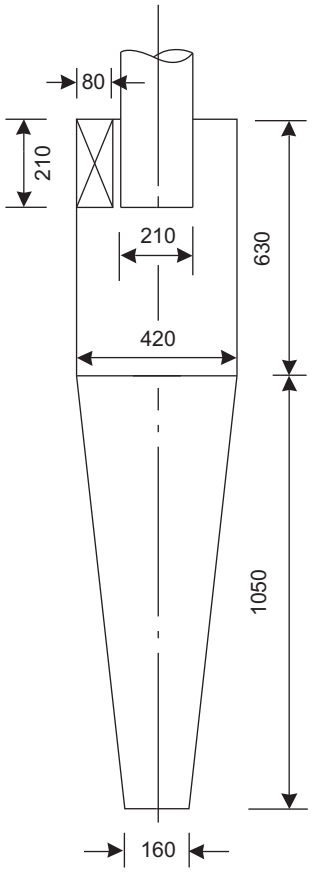


FIG. 18.36 Proposed cyclone design, all dimensions mm (Example 10.6).

18.5.4 Filters

The filters used for gas cleaning separate the solid particles by a combination of impingement and filtration; the pore sizes in the filter media used are too large simply to filter out the particles. The separating action relies on the precoating of the filter medium by the first particles separated, which are separated by impingement on the filter medium fibers. Woven or felted cloths of cotton and various synthetic fibers are commonly used as the filter media. Glass-fiber mats and paper filter elements are also used.

A typical example of this type of separator is the bag filter, which consists of a number of bags supported on a frame and housed in a large rectangular chamber (Fig. 18.37). The deposited solids are removed by mechanically vibrating the bag or by periodically reversing the gas flow. Bag filters can be used to separate small particles, down to around 1 μm, with a high separating efficiency. Commercial units are available to suit most applications and should be selected in consultation with a vendor.

The design and specification of bag filters (baghouses) is covered by Kraus (1979).

Air filters

Dust-free air is required for many process applications. The requirements of air filtration differ from those of process gas filtration mainly in that the quantity of dust to be removed will be lower, typically less than 10 mg/m^3 (~5 grains per 1000 ft^3), and also in that there is no requirement to recover the material collected.

Three basic types of air filters are used: viscous, dry, and continuous. Viscous and dry units are similar in construction, but the filter medium of the viscous type is coated with a viscous material, such as a mineral oil, to retain the dust. The filters are made up from standard, preformed, sections, supported on a frame in a filter housing. The sections are removed periodically for cleaning or replacement. Various designs of continuous filtration equipment are also available, employing either viscous or dry filter elements, but in which the filter is cleaned continuously. A comprehensive description of air filtration equipment is given by Strauss (1975).

18.5.5 Wet scrubbers (washing)

In wet scrubbing, the dust is removed by countercurrent washing with a liquid, usually water, and the solids are removed as a slurry. The principal mechanism involved is the impact (impingement) of the dust particles and the water droplets. Particle sizes down to 0.5 μm can be removed in suitably designed scrubbers. In addition to

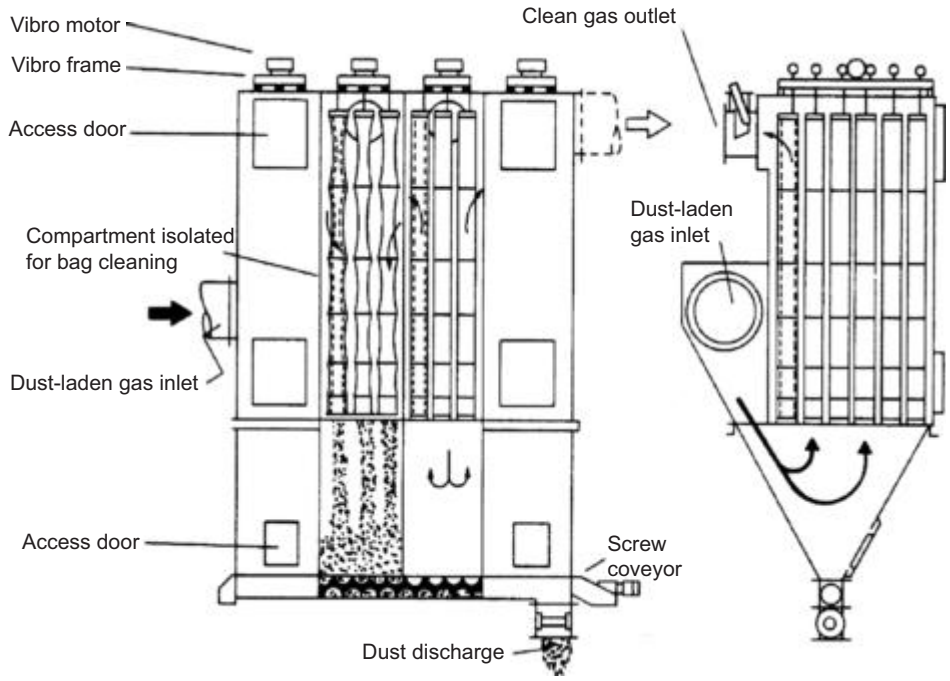


FIG. 18.37 Multicompartment vibro bag filter.

removing solids, wet scrubbers can be used to simultaneously cool the gas and neutralize any corrosive constituents.

Spray towers, plate, and packed columns are used, as well as a variety of proprietary designs. Spray towers have a low pressure drop but are not suitable for removing very fine particles, below 10 μm. The collecting efficiency can be improved by the use of plates or packing but at the expense of a higher pressure drop. A packed or plate column for wet scrubbing would typically be designed with three to five plates or height equivalent to three theoretical stages of packing.

Venturi and orifice scrubbers are simple forms of wet scrubbers. The turbulence created by the venturi or orifice is used to atomize water sprays and promote contact between the liquid droplets and dust particles. The agglomerated particles of dust and liquid are then collected in a centrifugal separator, usually a cyclone.

18.5.6 Electrostatic precipitators

Electrostatic precipitators are capable of collecting very fine particles, <2 μm, at high efficiencies; however, their capital and operating costs are high. Electrostatic precipitation should only be considered in place of alternative processes, such as filtration, where the gases are hot or corrosive.

Electrostatic precipitators are used extensively in the metallurgical, cement, and electrical power industries. Their main application is probably in the removal of the fine fly ash formed in the combustion of pulverized coal in power station boilers. The basic principle of operation is simple. The gas is ionized in passing between a high-voltage electrode and an earthed (grounded) electrode; the dust particles become charged and are attracted to the earthed electrode. The precipitated dust is removed from the electrodes mechanically, usually by vibration or by washing. Wires are normally used for the high-voltage electrode and plates or tubes for the earthed electrode. A typical design is shown in Fig. 18.38. A full description of the construction, design, and application of electrostatic precipitators is given by Schneider et al. (1975) and Parker (2002).

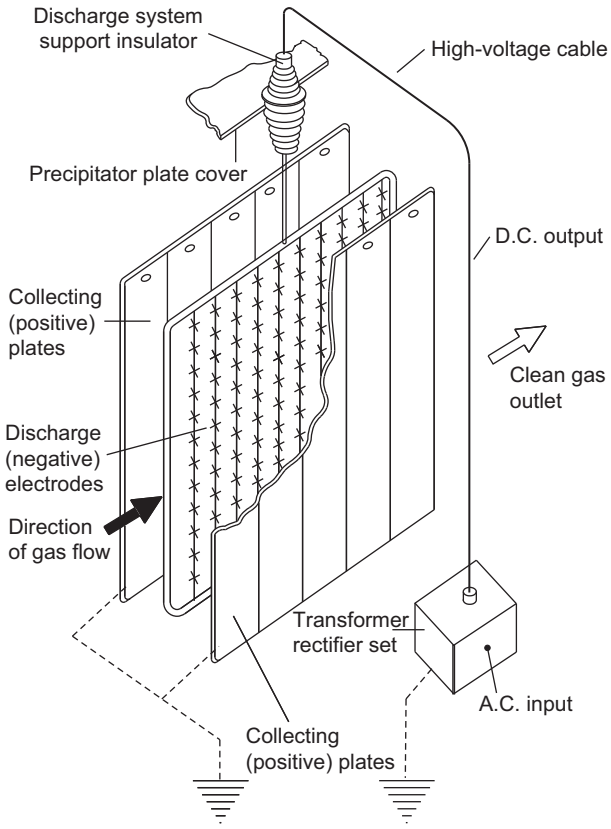


FIG. 18.38 Electrostatic precipitator.

18.6 Separation of solids from liquids

The need to separate solid and liquid phases is probably the most common phase separation requirement in the process industries, and many techniques are used (Fig. 18.39). The most suitable technique will depend on the solids concentration and feed rate, as well as the size and nature of the solid particles. The range of application of various techniques and equipment, as a function of slurry concentration and particle size, is shown in Fig. 18.40.

The choice of equipment also depends on whether the prime objective is to obtain a clear liquid or a solid product and on the degree of dryness of the solid required.

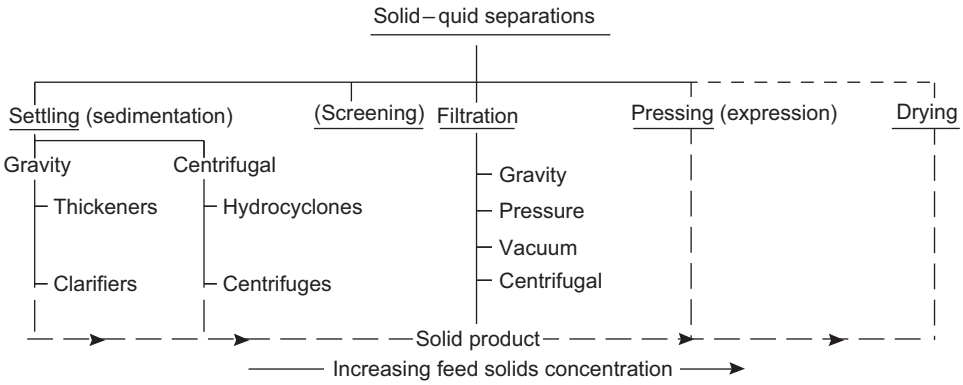


FIG. 18.39 Solid–liquid separation techniques.

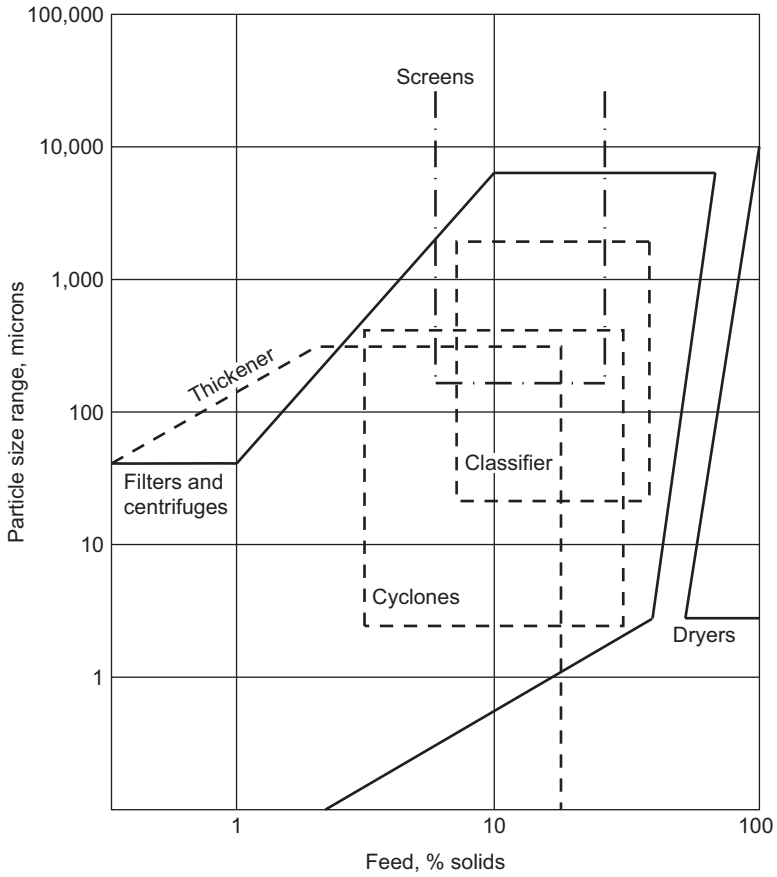


FIG. 18.40 Solid–liquid separation techniques. *(From Dahlstrom & Cornell, 1971.)*

The design, construction, and application of thickeners, centrifuges, and filters is a specialized subject, and firms that have expertise in these fields should be consulted when selecting and specifying equipment for new applications. Several specialist texts on the subject are available: Svarovsky (2001), Rushton et al. (2000), and Wakeman and Tarleton (1998). The theory of sedimentation processes and filtration is covered in Chhabra and Gurappa (2019).

18.6.1 Thickeners and clarifiers

Thickening and clarification are sedimentation processes, and the types of equipment used for the two techniques are similar. The primary purpose of thickening is to increase the concentration of a relatively large quantity of suspended solids, whereas that of clarifying, as the name implies, is to remove a small quantity of fine solids to produce a clear liquid effluent. Thickening and clarification are relatively cheap processes when used for the treatment of large volumes of liquid.

A thickener, or clarifier, consists essentially of a large circular tank with a rotating rake at the base. Rectangular tanks are also used, but the circular design is preferred. They can be classified according to the way the rake is supported and driven. The three basic designs are shown in Fig. 18.41. Various designs of rake are used, depending on the nature of the solids.

The design and construction of thickeners and clarifiers are described by Dahlstrom and Cornell (1971).

Flocculating agents are often added to promote the separating performance of thickeners.

18.6.2 Filtration

In filtration processes, the solids are separated from the liquid by passing (filtering) the slurry through some form of porous filter medium. Filtration is a widely used separation process in the chemical and other process industries. Many types of equipment and filter media are used, designed to meet the needs of particular applications.

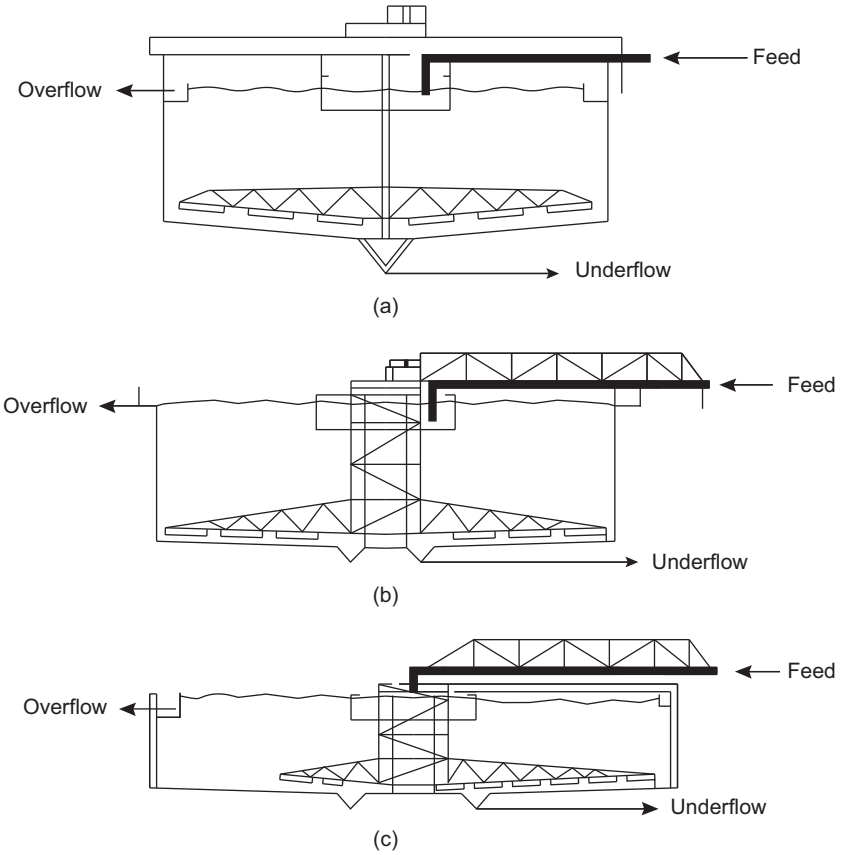


FIG. 18.41 Types of thickeners and clarifiers. (a) Bridge supported (up to <40 m dia.). (b) Center column supported (<30 m dia.). (c) Traction driven (<60 m dia.).

Descriptions of the filtration equipment used in the process industries and their fields of application can be found in various handbooks: Green and Southard (2018), Sparks and Chase (2015), and Schweitzer (1997) and in specialist texts on the subject: Cheremisinoff (1998), Orr (1977), Cheryan (2016), and Wakeman and Tarleton (2005). Biopharmaceutical applications are discussed in Jornitz (2019). A short discussion of filtration theory and descriptions of the principal types of equipment is given in Chhabra and Gurappa (2019).

The most commonly used filter medium is woven cloth, but many other media are also used. The main types are listed in Table 18.7. A comprehensive discussion of the factors to be considered when selecting filter media is given by Purchas (1971) and Mais (1971); see also Purchas and Sutherland (2001). Filter aids are often used to increase the rate of filtration of difficult slurries. They are either applied as a precoat to the filter cloth or added to the slurry and deposited with the solids, assisting in the formation of a porous cake.

Industrial filters use vacuum, pressure, or centrifugal force to drive the liquid (filtrate) through the deposited cake of solids. Filtration is essentially a discontinuous process. With batch filters, such as plate and frame presses, the equipment has to be shut down to discharge the cake, and even with those filters designed for continuous operation, such as rotating drum filters and cross-flow filters, periodic stoppages are necessary to change the filter cloths. Batch filters can be coupled to continuous plant by using several units in parallel or by providing buffer storage capacity for the feed and product.

The principal factors to be considered when selecting filtration equipment are:

1. The nature of the slurry and the cake formed
2. The solids concentration in the feed
3. The throughput required
4. The nature and physical properties of the liquid: viscosity, flammability, toxicity, corrosiveness
5. Whether cake washing is required
6. The cake dryness required
7. Whether contamination of the solid by a filter aid is acceptable
8. Whether the valuable product is the solid or the liquid, or both

The overriding factor will be the filtration characteristics of the slurry: whether it is fast filtering (low specific cake resistance) or slow filtering (high specific cake resistance). The filtration characteristics can be determined by laboratory or pilot plant tests. A guide to filter selection by the slurry characteristics is given in Table 18.8, which is based on a similar selection chart given by Porter et al. (1971).

The principal types of industrial-scale filters used are described briefly next.

Nutsche (gravity and vacuum operation)

This is the simplest type of batch filter. It consists of a tank with a perforated base, which supports the filter medium.

TABLE 18.7 Filter media

Type	Example	Minimum size particle trapped (μm)
1. Solid fabrication	Scalloped washers, wire-wound tubes	5
2. Rigid porous media	Ceramics, stoneware	1
	Sintered metal	3
3. Metal	Perforated sheets	100
	Woven wire	5
4. Porous plastics	Pads, sheets	3
	Membranes	0.005
5. Woven fabrics	Natural and synthetic fiber cloths	10
6. Nonwoven fabrics	Felts, lap	10
	Paper, cellulose	5
7. Cartridges	Yarn-wound spools, graded fibers	2
8. Loose solids	Fibers, asbestos, cellulose	Submicron

TABLE 18.8 Guide to filter selection

Slurry characteristics	Fast filtering	Medium filtering	Slow filtering	Dilute	Very dilute
Cake formation rate	cm/s	mm/s	0.02–0.12 mm/s	0.02 mm/s	No cake
Normal concentration	>20%	10–20%	1–10%	<5%	<0.1%
Settling rate	Very fast	Fast	Slow	Slow	—
Leaf test rate, kg/h m^2	>2500	250–2500	25–250	<25	—
Filtrate rate, $m^3/h\ m^2$	>10	5–10	0.02–0.05	0.02–5	0.02–5
Filter application					
Continuous vacuum filters					
Multicompartment drum	■	■	■		
Single compartment drum	■	■			
Top feed drum	■	■			
Scroll discharge drum	■	■	■		
Tilting pan	■	■	■		
Belt	■	■	■		
Disc		■	■		
Batch vacuum leaf		■	■	■	■
Batch nutsche	■	■	■	■	■
Batch pressure filters					
Plate and frame		■	■	■	■
Vertical leaf		■	■	■	■
Horizontal plate	■	■	■	■	■
Cartridge edge					■

Plate and frame press (pressure operation) (Fig. 18.42)

These are the oldest and most commonly used batch filters. The equipment is versatile, made in a variety of materials, and capable of handling viscous liquids and cakes with a high specific resistance.

Leaf filters (pressure and vacuum operation)

Various types of leaf filters are used, with the leaves arranged in horizontal or vertical rows. The leaves consist of metal frames over which filter cloths are draped. The cake is removed either mechanically or by sluicing it off with jets of water. Leaf filters are used for similar applications as plate and frame presses, but generally have lower operating costs.

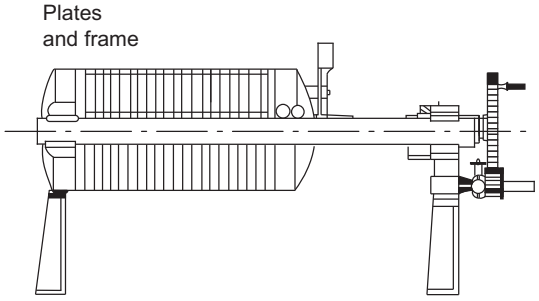


FIG. 18.42 Plate and frame filter press.

Rotary drum filters (usually vacuum operation) (Fig. 18.43)

A drum filter consists essentially of a large hollow drum around which the filter medium is fitted. The drum is partially submerged in a trough of slurry, and the filtrate is sucked through the filter medium by vacuum inside the drum. Wash water can be sprayed on to the drum surface, and multicompartment drums are used so that the wash water can be kept separate from the filtrate. A variety of methods are used to remove the cake from the drum: knives, strings, air jets, and wires. Rotating drum filters are essentially continuous in operation. They can handle large throughputs and are widely used for free-filtering slurries.

Disc filters (pressure and vacuum operation)

Disc filters are similar in principle to rotary filters, but consist of several thin discs mounted on a shaft, in place of the drum. This gives a larger effective filtering area on a given floor area, and vacuum disc filters are used in preference to drum filters where space is restricted. At sizes above approximately 25 m^2 filtration area, disc filters are cheaper, but their applications are more restricted, as they are not as suitable for the application of wash water or precoating.

Belt filters (vacuum operation) (Fig. 18.44)

A belt filter consists of an endless reinforced rubber belt with drainage holes along its center, which supports the filter medium. The belt passes over a stationary suction box into which the filtrate is sucked. Slurry and wash water are sprayed on to the top of the belt.

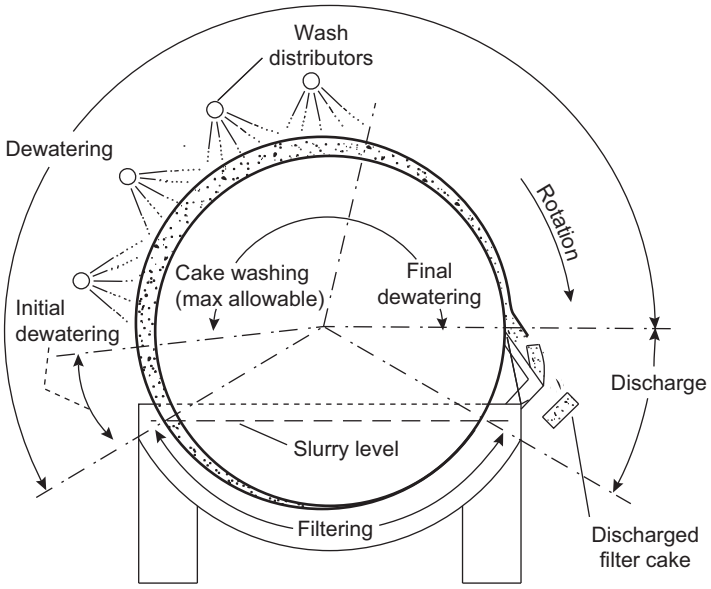


FIG. 18.43 Drum filter.

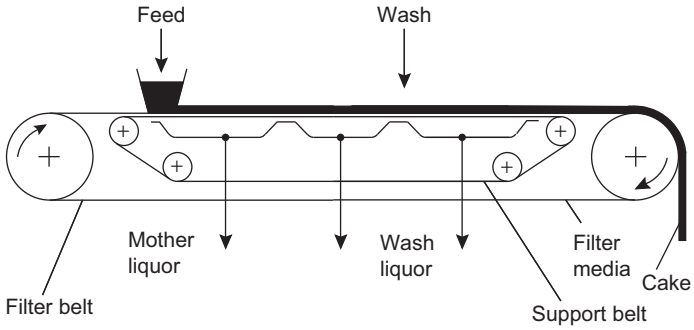


FIG. 18.44 Belt filter.

Horizontal pan filters (vacuum operation) (Fig. 18.45)

This type is similar in operation to a vacuum Nutsche filter. It consists of shallow pans with perforated bases, which support the filter medium. By arranging a series of pans around the circumference of a rotating wheel, the operation of filtering, washing, drying, and discharging can be made automatic.

Centrifugal filters

Centrifugal filters use centrifugal force to drive the filtrate through the filter cake. The equipment used is described in the next section.

Cross-flow filters

Cross-flow filters are used to reject liquid from a slurry, similar to thickeners. The filter is arranged as tubular modules and is often a porous membrane; see Section 16.5.4. The slurry is usually fed through the tubes and clear liquid is withdrawn through the tube wall as filtrate, as illustrated in Fig. 18.46. The flow on the inside of the tube prevents the accumulation of solids, and the concentrated slurry can then be sent for further processing.

Cross-flow filtration for solvent rejection is often carried out in a "feed and bleed" flow scheme, shown in Fig. 18.47. A portion of the retentate from the filtration unit is recycled to the feed. This flow scheme allows higher velocities to be used on the retentate side, and hence higher concentrations can be reached without fouling the filter surface.

Cross-flow filtration processes such as microfiltration and ultrafiltration are widely used in food processing, for example, in concentrating orange juice, and also in the recovery of products from fermentation processes. See Harrison (2014) and Gabelman (2017) for examples.

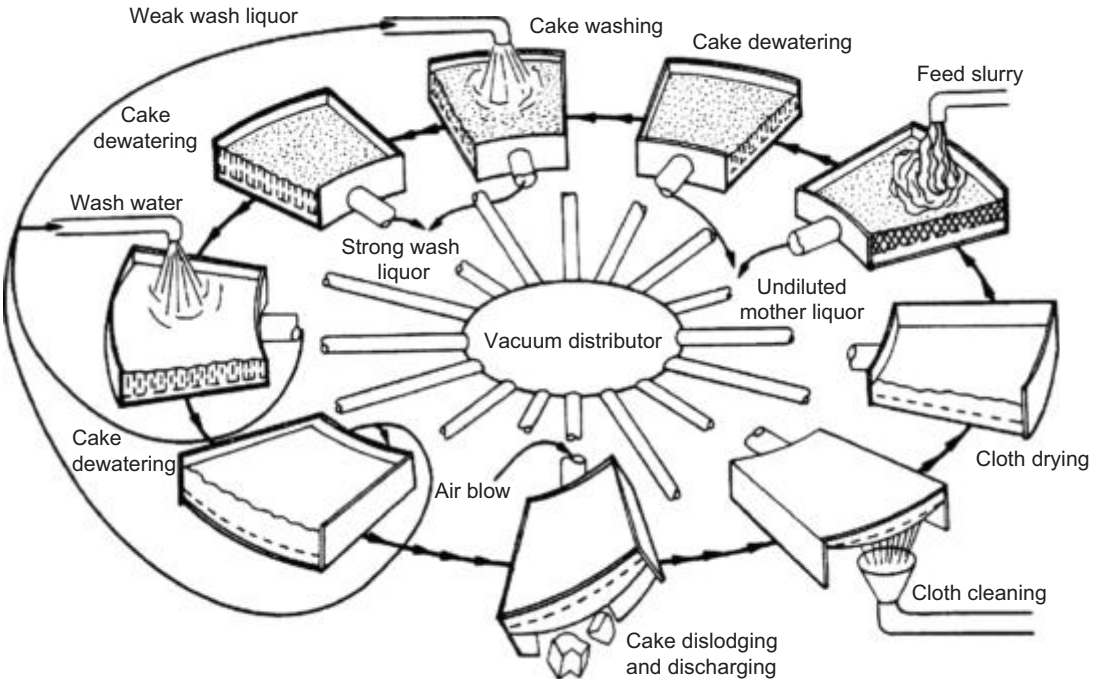


FIG. 18.45 Pan filters.

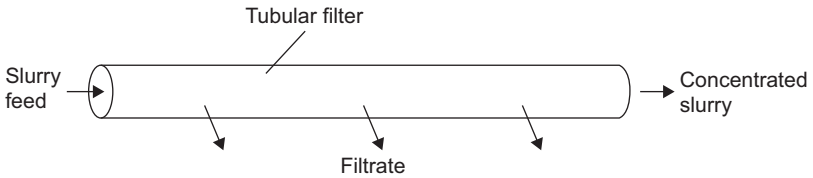


FIG. 18.46 Cross-flow filtration.

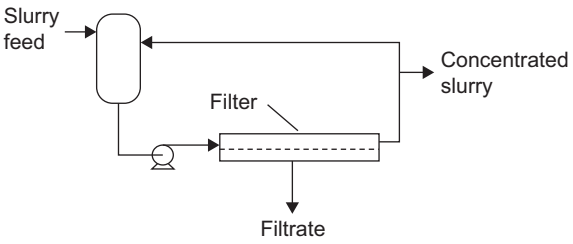


FIG. 18.47 Feed and bleed filtration.

18.6.3 Centrifuges

Centrifuges are classified according to the mechanism used for solids separation:

1. Sedimentation centrifuges, in which the separation is dependent on a difference in density between the solid and liquid phases (solid heavier).
2. Filtration centrifuges, which separate the phases by filtration. The walls of the centrifuge basket are porous, and the liquid filters through the deposited cake of solids and is removed.

The choice between a sedimentation or filtration centrifuge for a particular application will depend on the nature of the feed and the product requirements. The main factors to be considered are summarized in Table 18.9. As a general rule, sedimentation centrifuges are used when a clarified liquid product is required, and filtration centrifuges to produce a pure, dry, solid product.

A variety of centrifugal filter and sedimenter designs are used. The main types are listed in Table 18.10. They can be classified by a number of design and operating features, such as:

1. Mode of operation — batch or continuous
2. Orientation of the bowl/basket — horizontal or vertical
3. Position of the suspension and drive — overhung or underhung
4. Type of bowl — solid, perforated basket, disc bowl
5. Method of solids cake removal
6. Method of liquid removal

Descriptions of the various types of centrifuges and their fields of application can be found in various handbooks; in a book by Leung (1998); and in articles by Ambler (1971), Linley (1984), and Patnaik (2012).

The fields of application of each type, classified by the size range of the solid particles separated, are given in Fig. 18.48. A similar selection chart is given by Schroeder (1998).

Sedimentation centrifuges

There are four main types of sedimentation centrifuges:

TABLE 18.9 Selection of sedimentation or filter centrifuge

Factor	Sedimentation	Filtration
Solids size, fine		x
Solids size, >150 μm	x	
Compressible cakes	x	
Open cakes		x
Dry cake required		x
High filtrate clarity	x	
Crystal breakage problems		x
Pressure operation		
High-temperature	will depend on the type of operation centrifuge used	

TABLE 18.10 Centrifuge types

Sedimentation	Filtration-fixed bed
Laboratory	Vertical basket
Bottle	Manual discharge
Ultra	Bag discharge
	Knife discharge
Tubular bowl	Horizontal basket
	Inclined basket
Disc	
Batch bowl	
Nozzle discharge	
Valve discharge	Filtration-moving bed
Opening bowl	
Imperforate basket	Conical bowl
Manual discharge	Wide angle
Skimmer discharge	Vibrating
	Torsional
	Tumbling
Scroll discharge	Scroll discharge
Horizontal	
Cantilevered	Cylindrical bowl
Vertical	Scroll discharge
Screen bowl	Pusher

From Sutherland (1970)

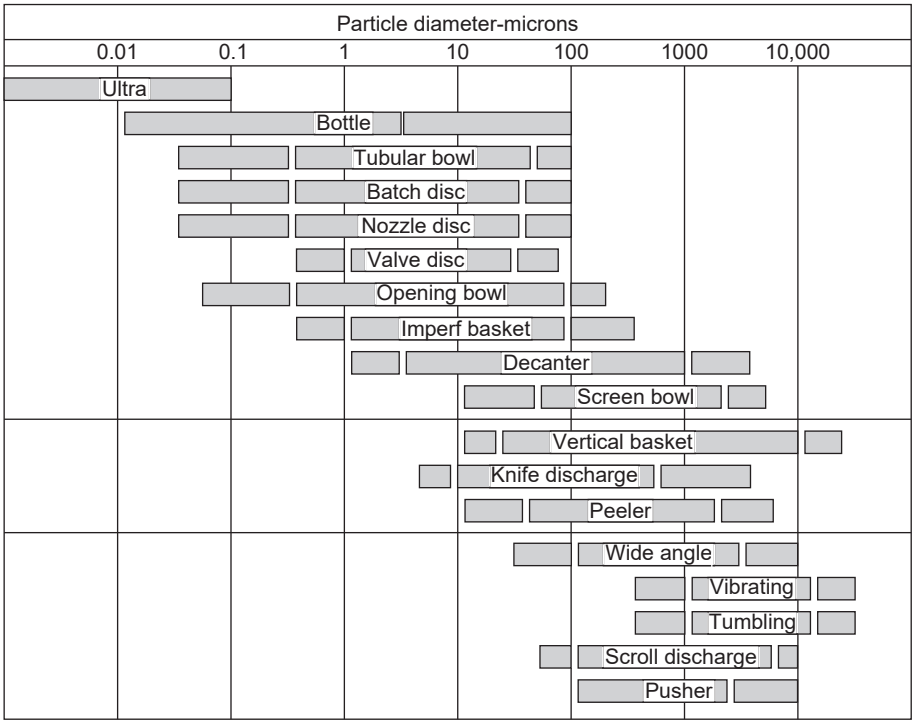


FIG. 18.48 Classification of centrifuges by particle size. *(From Sutherland, K. S. [1970]. How to specify a centrifuge.* Chemical Processing, *16[May], 10.)*

1. Tubular bowl (Fig. 18.49)

High-speed, vertical-axis, tubular bowl centrifuges are used for the separation of immiscible liquids, such as water and oil, and for the separation of fine solids. The bowl is driven at speeds of around 15,000 rpm (250 Hz), and the centrifugal force generated exceeds 130,000 N.

2. Disc bowl (Fig. 18.50)

The conical discs in a disc bowl centrifuge split the liquid flow into a number of very thin layers, which greatly increases the separating efficiency. Disc bowl centrifuges are used for separating liquids and fine solids and for solids classification.

3. Scroll discharge

In this type of machine, the solids deposited on the wall of the bowl are removed by a scroll (a helical screw conveyer), which revolves at a slightly different speed from the bowl. Scroll discharge centrifuges can be designed so that solids can be washed and relatively dry solids can be discharged.

4. Solid bowl batch centrifuge

The simplest type; similar to the tubular bowl machine, but with a smaller bowl length-to-diameter ratio (less than 0.75).

The tubular bowl type is rarely used for solids concentrations above 1% by volume. For concentrations between 1% and 15%, any of the other three types can be used. Above 15%, either the scroll discharge type or the batch type may be used, depending on whether continuous or intermittent operation is required.

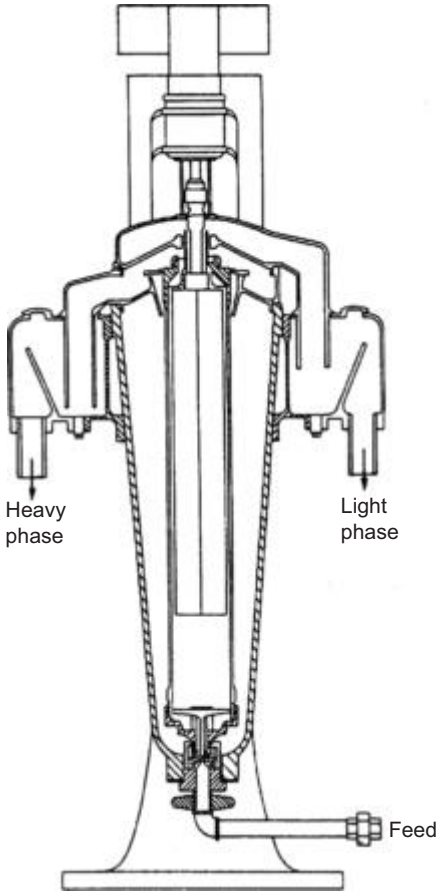


FIG. 18.49 Tubular bowl centrifuge.

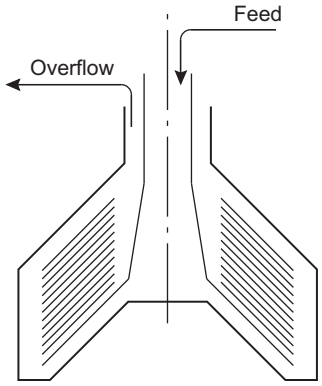


FIG. 18.50 Disc bowl centrifuge.

Sigma theory for sedimentation centrifuges

The basic equations describing sedimentation in a centrifugal field are given in Chhabra and Gurappa (2019). In that discussion the term *sigma* (Σ) is introduced, which can be used to define the performance of a centrifuge independently of the physical properties of the solid–fluid system. The sigma value of a centrifuge, normally expressed in cm^2, is equal to the cross-sectional area of a gravity settling tank having the same clarifying capacity.

This approach to describing centrifuge performance has become known as the "sigma theory." It provides a means for comparing the performance of sedimentation centrifuges and for scaling up from laboratory and pilot-scale tests; see Ambler (1952) and Trowbridge (1962).

In the general case, it can be shown that:

$$Q = 2u_g\Sigma \tag{18.25}$$

and (where Stokes law applies)

$$u_g = \frac{\Delta\rho d_s^2 g}{18\mu} \tag{18.26}$$

Note: The factor of 2 is included in Equation 18.25, as d_s is the *cut-off* size; 50% of particles of this size will be removed in passage through the centrifuge.

where Q = volumetric flow of liquid through the centrifuge, m^3/s
u_g = terminal velocity of the solid particle settling under gravity through the liquid, m/s
Σ = sigma value of the centrifuge, m^2
$\Delta\rho$ = density difference between solid and liquid, kg/m^3
d_s = the diameter of the solid particle, *the cut-off* size, m ($\mu m \times 10^{-6}$)
μ = viscosity of the liquid, $Nm^{-2}s$
g = gravitational acceleration, 9.81 m/s^2

Morris (1966) gives a method for the selection of the appropriate type of sedimentation centrifuge for a particular application based on the ratio of the liquid overflow to sigma value (Q/Σ). His values for the operating range of each type, and their approximate efficiency rating, are given in Table 18.11. The efficiency term is used to account for the different amounts by which the various designs differ from the theoretical sigma values given by Equation 18.25. Sigma values depend solely on the geometrical configuration and speed of the centrifuge. Details of the calculation for various types are given by Ambler (1952). To use Table 18.11, it is necessary to know the feed rate of slurry (and hence the liquid overflow Q), the density of the liquid and solid, the liquid viscosity, and the diameter of the particle for, say, a 98% size removal. The use of Table 18.11 is illustrated in Example 18.3.

TABLE 18.11 Selection of sedimentation centrifuges

Type	Approximate efficiency (%)	Normal operating range Q, m^3/h at Q/Σ m/s
Tubular bowl	90	0.4 at 5×10^{-8} to 4 at 3.5×10^{-7}
Disc	45	0.1 at 7×10^{-8} to 110 at 4.5×10^{-7}
Solid bowl (scroll discharge)	60	0.7 at 1.5×10^{-6} to 15 at 1.5×10^{-5}
Solid bowl (basket)	75	0.4 at 5×10^{-6} to 4 at 1.5×10^{-4}

A selection guide for sedimentation centrifuges by Lavanchy et al. (1964), which includes other types of solid–liquid separators, is shown in Fig. 18.51, adapted to SI units.

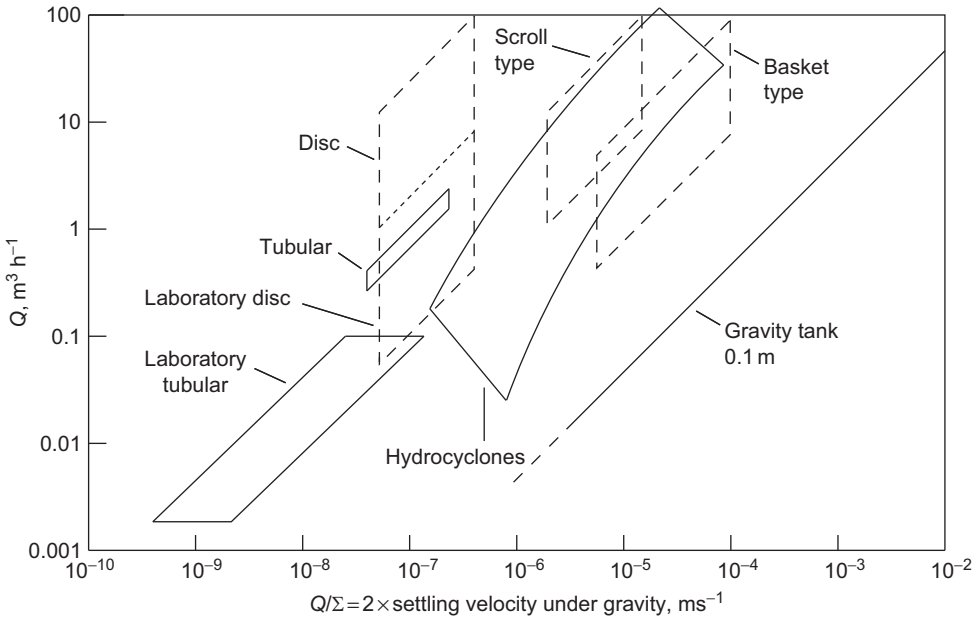


FIG. 18.51 Performance of sedimentation equipment. *(From Lavanchy, A. C., Keith, F. W. , & Beams, J. W. [1964]. Centrifugal separation. In* Kirk-Othmer encyclopedia of chemical technology, *2nd ed. Interscience.)*

Example 18.3

A precipitate is to be continuously separated from a slurry. The solids concentration is 5% and the slurry feed rate 5.5 m^3/h. The relevant physical properties at the system operating temperature are:

liquid density 1050 kg/m^3, viscosity 4 cP $(mNm^{-2}s)$,

solid density 2300 kg/m^3, "cut-off" particle size 10μm $= 10 \times 10^{-6}$m.

Solution

$$\text{Overflow rate, } Q = 0.95 \times 5.5 = 5.23 \text{ m}^3/\text{h}$$

$$= \frac{5.13}{3600} = 1.45 \times 10^{-3} \text{ m}^3/\text{s}$$

$$\Delta\rho = 2300 - 1050 = 1250 \text{ kg/m}^3$$

From Equations 18.25 and 18.26:

$$\frac{Q}{\Sigma} = 2 \times \frac{1250(10 \times 10^{-6})^2}{18 \times 4 \times 10^{-3}} \times 9.81 = 3.4 \times 10^{-5}$$

From Table 18.11, for a Q of 5.23 m^3/h at a Q/Σ of 3.4×10^{-5}, a solid bowl basket type should be used.

To obtain an idea of the size of the machine needed, the sigma value can be calculated using the efficiency value from Table 18.11.

From Equation 18.25:

$$\Sigma = \frac{Q}{eff. \times 2u_g} = \frac{1.45 \times 10^{-3}}{0.75 \times 3.4 \times 10^{-5}}$$

$$= \underline{56.9 \text{ m}^2}$$

The sigma value is the equivalent area of a gravity settler that would perform the same separation as the centrifuge. Once the sigma value is known, a suitable machine can be selected by reviewing performance data on manufacturers' websites.

Filtration centrifuges (centrifugal filters)

It is convenient to classify centrifugal filters into two broad classes, depending on how the solids are removed: fixed bed or moving bed.

In the fixed-bed type, the cake of solids remains on the walls of the bowl until removed either manually or automatically by means of a knife mechanism. It is essentially cyclic in operation. In the moving-bed type, the mass of solids is moved along the bowl by the action of a scroll (similar to the solid-bowl sedimentation type), or by a ram (pusher type), or by a vibration mechanism, or by the bowl angle. Washing and drying zones can be incorporated into the moving-bed type.

Bradley (1965) has grouped the various types into the family tree shown in Fig. 18.52.

Schematic diagrams of the various types are shown in Fig. 18.53. The simplest machines are the basket types (Fig. 18.53a, b, and c), and these form the basic design from which the other types have been developed (Fig. 18.53d to o).

The various arrangements of knife mechanisms used for automatic removal of the cake are shown in Fig. 18.53(d) to (h). The bottom discharge-type machines (Fig. 18.53d and e) can be designed for variable-speed automatic

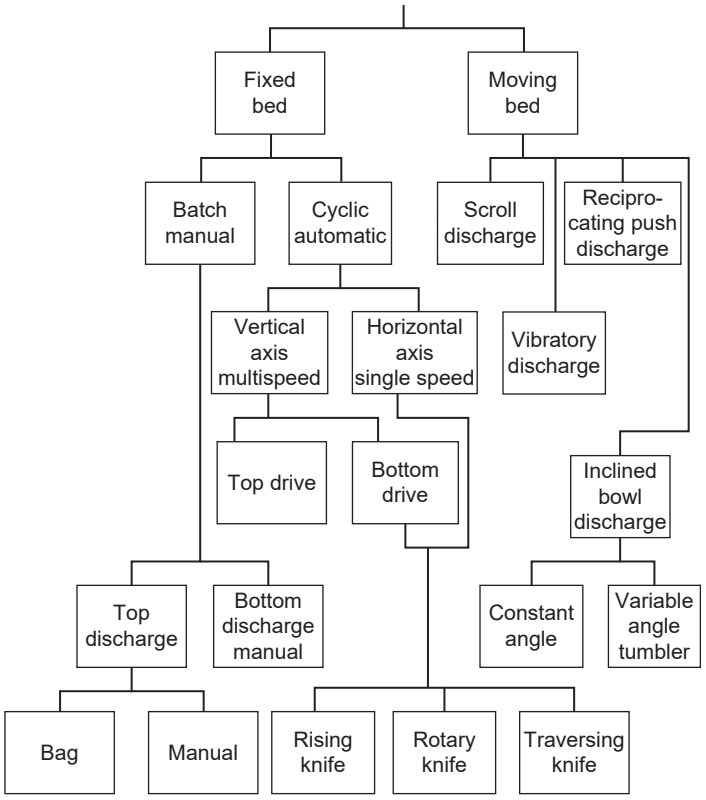


FIG. 18.52 Filtration centrifuge family tree. *(From Bradley, D. [1965]. Medium-speed centrifuges.* Chemical and Process Engineering, *595.)*

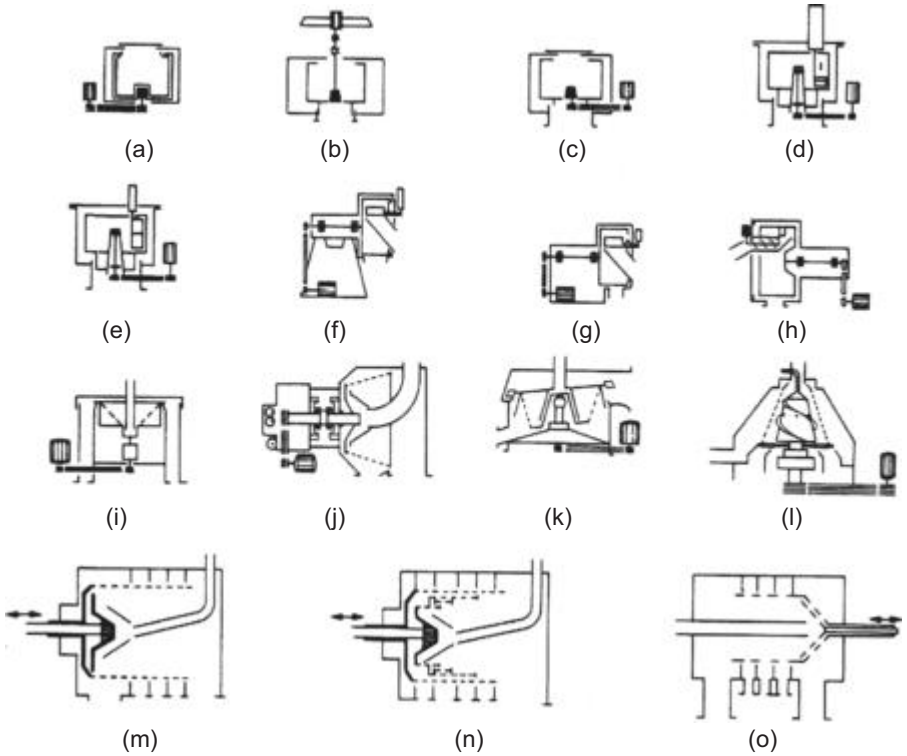


FIG. 18.53 Schematic diagrams of filtration centrifuge types. (a) Bottom drive batch basket with bag. (b) Top drive bottom discharge batch basket. (c) Bottom drive bottom discharge batch basket. (d) Bottom drive automatic basket, rising knife. (e) Bottom drive automatic basket, rotary knife. (f) Single reversing knife rising knife. (g) Single-speed automatic rotary knife. (h) Single-speed automatic traversing knife. (i) Inclined wall self-discharge. (j) Inclined vibrating wall self-discharge. (k) Inclined "tumbling" wall self-discharge. (l) Inclined wall scroll discharge. (m) Traditional single-stage pusher. (n) Traditional multistage pusher. (o) Conical pusher with de-watering cone. *(From Bradley, 1965.)*

discharge and are suitable for use with fragile or plate or needle-shaped crystals, where it is desirable to avoid breakage or compaction of the bed. They can be loaded and discharged at low speeds, which reduces breakage and compaction of the cake. The single-speed machines (Fig. 18.53f, g, and h) are used where cakes are thin and short cycle times are required. They can be designed for high-temperature and high-pressure operation. When continuous operation is required, the scroll, pusher, or other self-discharge types are used (Fig. 18.53i to o). The scroll discharge centrifuge is a low-cost, flexible machine, capable of a wide range of applications but is not suitable for handling fragile materials. It is normally used for coarse particles, where some contamination of the filtrate with fines can be tolerated.

The capacity of filtration centrifuges is highly dependent on the solids concentration in the feed. For example, at 10% feed slurry concentration, 9 kg of liquid will be centrifuged for every 1 kg of solids separated, whereas with a 50% solids concentration, the quantity will be less than 1 kg. For dilute slurries it is well worth considering using some form of preconcentration, such as gravity sedimentation, hydrocyclones, or cross-flow filtration.

18.6.4 Hydrocyclones (liquid cyclones)

Hydrocyclones are used for solid−liquid separations as well as for solids classification and liquid−liquid separation. A hydrocyclone is a centrifugal device with a stationary wall, with the centrifugal force being generated by the liquid motion. The operating principle is basically the same as that of the gas cyclone described in Section 18.5.3. Hydrocyclones are simple, robust separating devices that can be used over the particle size range from 4 to 500 μm. They are often used in groups, as illustrated in Fig. 18.54. The design and application of hydrocyclones is discussed fully in books by Abulnaga (2002) and Svarovsky and Thew (1992). Design methods and charts are also given by Zanker (1977), Day et al. (1997), and Moir (1985).

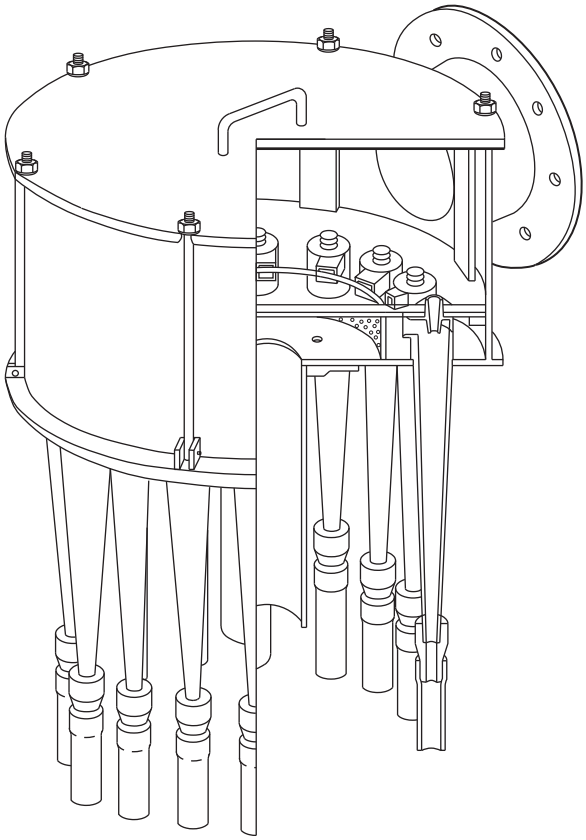


FIG. 18.54 A "clog" assembly of 16 × 2 in (50 mm) diameter hydrocyclone. *(Courtesy of Richard Mozley Ltd.)*

The nomographs by Zanker can be used to make a preliminary estimate of the size of cyclone needed. The specialist manufacturers of hydrocyclone equipment should be consulted to determine the best arrangements and design for a particular application.

Zanker's method is outlined here and illustrated in Example 18.4. Fig. 18.56 is based on an empirical equation by Bradley (1960):

$$d_{50} = 4.5\left[\frac{D_c^3 \mu}{L^{1.2}(\rho_s - \rho_L)}\right] \tag{18.27}$$

where d_{50} = the particle diameter for which the cyclone is 50% efficient, μm
D_c = diameter of the cyclone chamber, cm
μ = liquid viscosity, centipoise (mN s/m^2)
L = feed flow rate, l/min
ρ_L = density of the liquid, g/cm^3
ρ_s = density of the solid, g/cm^3

The equation gives the chamber diameter required to separate the so-called d_{50} particle diameter as a function of the slurry flow rate and the liquid and solid physical properties. The d_{50} particle diameter is the diameter of the particle, 50% of which will appear in the overflow and 50% in the underflow. The separating efficiency for other particles is related to the d_{50} diameter by Fig. 18.55, which is based on a formula by Bennett (1936).

$$\eta = 100\left[1 - e^{-(d/d_{50} - 0.115)^3}\right] \tag{18.28}$$

where η = the efficiency of the cyclone in separating any particle of diameter d, percent
d = the selected particle diameter, μm

The method applies to hydrocyclones with the proportions shown in Fig. 18.57.

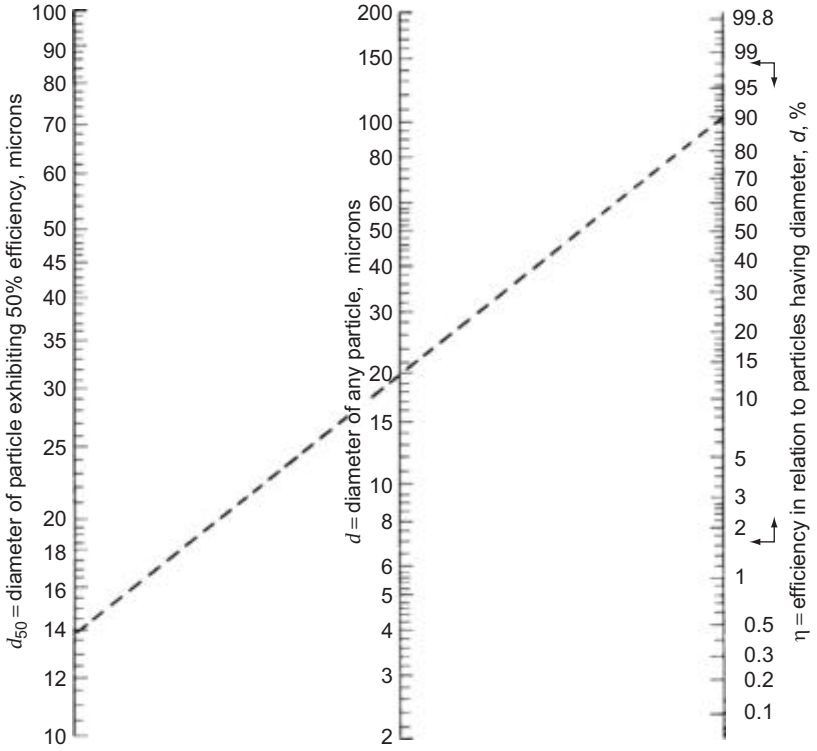


FIG. 18.55 Determination of d_{50} from the desired particle separation (Equation 18.27, Example 18.4). *(From Zanker, 1977.)*

Example 18.4

Estimate the size of hydrocyclone needed to separate 90% of particles with a diameter greater than 20 μm from 10 m^3/h of a dilute slurry.

Physical properties: solid density 2000 kg/m^3, liquid density 1000 kg/m^3, viscosity 1 mN s/m^2.

Solution

$$\text{Flow rate} = \frac{10 \times 10^3}{60} = 1.66.71/\text{min}$$

$$(\rho_s - \rho_L) = 2.0 - 1.0 = 1.0 \ \text{g/cm}^3$$

From Fig. 18.55, for 90% removal of particles above 20 μm:

$$d_{50} = 14 \ \mu\text{m}$$

From Fig. 18.56, for $\mu = 1$ mN s/m^2, $(\rho_s - \rho_L) = 1.0$ g/cm^3, $L = 167$/min

$$D_c = \underline{16 \text{ cm}}$$

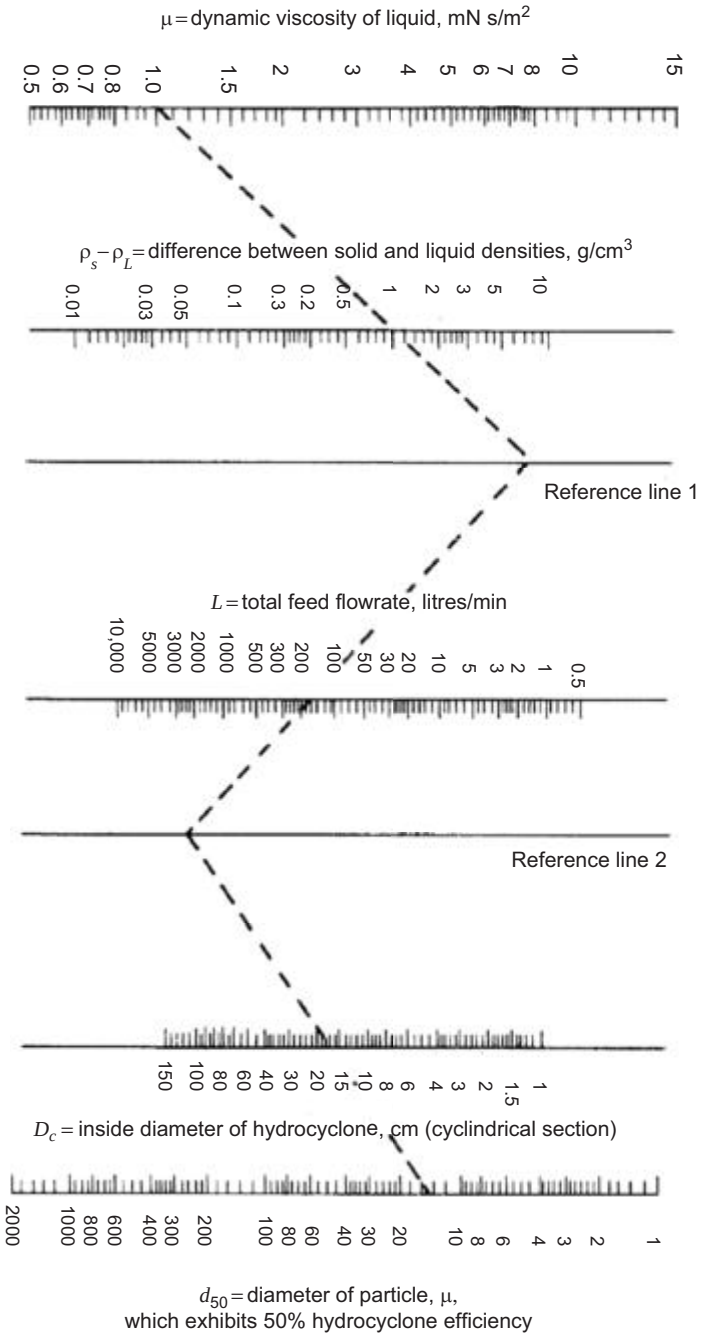


FIG. 18.56 Chamber dia. D_c from flow rate, physical properties, and d_{50} particle size (Equation 18.28, Example 18.4). *(From Zanker, 1977.)*

8.6.5 Pressing (expression)

Pressing, in which the liquid is squeezed (expressed) from a mass of solids by compression, is used for certain specialized applications. Pressing consumes a great deal of energy and should not be used unless no other separating technique is suitable; however, in some applications dewatering by pressing can be competitive with drying.

Presses are of two basic types: hydraulic batch presses and screw presses. Hydraulic presses are used for extracting fruit juices, and screw presses for dewatering materials such as paper pulp, garbage, and manure. The equipment used is described in Green and Southard (2018).

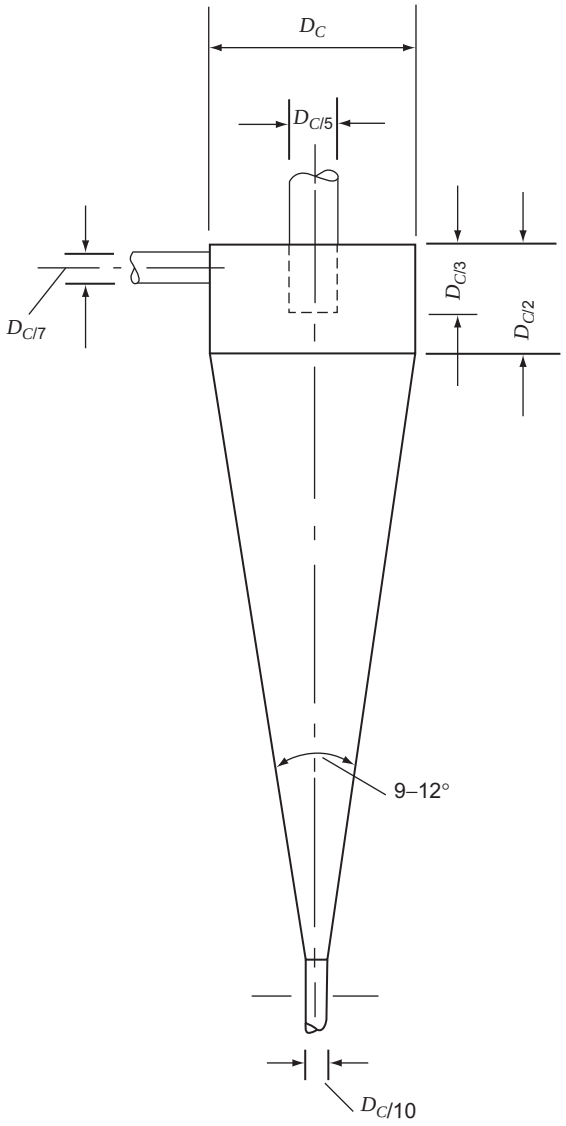


FIG. 18.57 Hydrocyclone-typical proportions.

18.7 Separation of liquids from solids (drying)

Drying is the removal of water, or other volatile liquids, by evaporation. Most solid materials require drying at some stage in their production. The choice of suitable drying equipment often cannot be separated from the selection of the upstream equipment feeding the drying stage.

The overriding consideration in the selection of drying equipment is the nature and concentration of the feed. Drying is an energy-intensive process, and the removal of liquid by thermal drying will be more costly than by mechanical separation techniques.

Drying equipment can be classified according to the following design and operating features:

1. Batch or continuous
2. Physical state of the feed: liquid, slurry, wet solid
3. Method of conveyance of the solid: belt, rotary, fluidized
4. Heating system: conduction, convection, radiation

Hot air is usually used as the heating and mass transfer medium in industrial dryers unless there are concerns about solvent flammability, in which case nitrogen, depleted air, or recirculating flue gas are used. The air may be directly

heated by firing a burner into the air stream (using oil, gas, or coal as fuel) or indirectly heated, usually by banks of steam-heated finned tubes. The heated air is usually propelled through the dryer by electrically driven fans.

Table 18.12, adapted from a similar selection guide by Parker (1963), shows the basic features of the various types of solids dryers used in the process industries; Table 18.13, by Williams-Gardner (1965), shows typical applications.

Batch dryers are normally used for small-scale production and when the drying cycle is likely to be long. Continuous dryers require less labor and less floor space and produce a more uniform quality product.

It is important to present the material to the dryer in a form that will produce a bed of solids with an open, porous structure. For pastes and slurries, some form of pretreatment equipment will normally be needed, such as extrusion or granulation.

Liquids can also be extracted from solids by leaching; see Section 16.5.6.

TABLE 18.12 Dryer selection

Mode of operation	Generic type	Feed condition 1	Feed condition 2	Feed condition 3	Specific dryer types	Jacketed	Suitable for heat-sensitive materials	Suitable for vacuum service	Retention or cycle time	Heat transfer method	Capacity	Typical evaporation capacity	
Batch	Stationary		↔	↔	1. Shelf 2. Cabinet 3. Compartment	Yes	Yes	Yes	6.48 h	Radiant and conduction	Limited	0.15–1.0	kg/hm² heat transfer area
			↔	↔	Truck	No	Yes	No	6.48 h	Convection	Limited	0.15–1.0	
		↔	↔		1. Kettle 2. Pan	Yes	No	Yes	3.12 h	Conduction	Limited	1.5–15	
			↔		Rotary shell	Yes	Yes	Yes	4.48 h	Conduction	Limited	0.5–12	
			↔		Rotary internal	Yes	Yes	Yes	4.48 h	Conduction	Limited	0.5–12	
			↔		Double cone	Yes	Yes	Yes	3.12 h	Conduction	Limited	0.5–12	
Continuous	Drum	↔			1. Single drum 2. Double drum 3. Twin drum	No	Yes	Yes	Very short	Conduction	Medium	5–50	
	Rotary		↔		Rotary direct heat	No	No	No	Long	Convection	High	3–110	kg/hm³ dryer volume
			↔		Rotary, indirect heat	No	No	No	Long	Conduction	Medium	15–200	
			↔		Rotary, steam tube	No	Depends on material	No	Long	Conduction	High	15–200	
			↔		Rotary, direct-indirect heat	No	No	No	Long	Conduction Convection	High	50–150	
			↔		Louver	No	Depends on material	No	Long	Convection	High	5–240	
			↔	↔	Tunnel belt, screen	No	Yes	No	Long	Convection	Medium	1.5–35	
	Conveyor		↔		Rotary shelf	Yes	Depends on material	No	Medium	Conduction Convection	Medium	0.5–10	kg/hm²
			↔		Trough	Yes	Depends on material	Yes	Varies	Conduction	Medium	0.5–15	
			↔		Vibrating	Yes	Depends on material	No	Medium	Convection Conduction	Medium	0.5–100	
			↔		Turbo	No	Depends on material	No	Medium	Convection	Medium	1–10	
	Suspended particle	↔			Spray	No	Yes	No	Short	Convection	High	1.5–50	kg/hm³
			↔		Flash	No	Yes	No	Short	Convection	High	–	
			↔		Fluid bed	No	Yes	No	Short	Convection	Medium	–	

↔ = applicable to feed conditions noted

Key to feed conditions:

1. Solutions, colloidal suspensions and emulsions, pumpable solids suspensions, pastes and sludges.
2. Free-flowing powders, granular, crystalline or fibrous solids that can withstand mechanical handling.
3. Solids incapable of withstanding mechanical handling.

TABLE 18.13 Dryer applications

Dryer type	System	Feed form	Typical products
Batch ovens	Forced convection	Paste, granules, extrude cake	Pigment dyestuffs, pharmaceuticals, fibers
	Vacuum	Extrude cake	Pharmaceuticals
" pan (agitated)	Atmospheric and vacuum	Crystals, granules, powders	Fine chemicals, food products
" rotary	Vacuum	Crystals, granules solvent recovery	Pharmaceuticals
" fluid bed	Forced convection	Granular, crystals	Fine chemicals, pharmaceuticals, plastics
" infrared	Radiant	Components sheets	Metal products, plastics
Continuous rotary	Convection Direct/indirect Direct Indirect Conduction	Crystals, coarse powders, extrudes preformed cake lumps, granular paste and fillers cakes back-mixed with dry product	Chemical ores, food products, clays, pigments, chemicals Carbon black
" film drum	Conduction	Liquids, suspensions	Foodstuffs, pigment
" trough	Conduction		Ceramics, adhesives
" spray	Convection	Liquids, suspensions	Foodstuffs, pharmaceuticals, ceramics, fine chemicals, detergents, organic extracts
" band	Convection	Preformed solids	Foodstuffs, pigments, chemicals, rubber, clays, ores, textiles
" fluid bed	Convection	Preformed solids granules, crystals	Ores, coal, clays, chemicals
" pneumatic	Convection	Preformed pastes, granules, crystals, coarse products	Chemicals, starch, flour, resins, wood-products, food products
" infra-red	Convection	Components sheets	Metal products, moulded fiber articles, painted surfaces

18.7.1 Theory of drying

Drying involves a combination of heat transfer and mass transfer. Heat is transferred to the surface of the solid to provide the heat of vaporization. The liquid evaporates and diffuses away from the surface into the bulk of the drying gas. Most dryers use a flowing gas to ensure that there is always an adequate partial pressure driving force for evaporation. Convective heat transfer is important in all dryers, although some designs also use conduction and radiation to increase the heating rate.

Much of the terminology used in drying refers to air–water systems, as these are widely encountered in the food, paper, textile, and minerals-processing industries. The same concepts can be extended to other liquids or solvents and to other drying gases.

The amount of drying that can be achieved depends on the nature of the solid and the moisture (or solvent) content of the inlet air (or gas). Nonporous solids such as sand can be dried to near-zero moisture regardless of the inlet gas condition. Porous solids, cellular and fibrous materials, and hygroscopic solids will reach a moisture content that is in equilibrium with the humidity of the entering gas. Consequently, to reach the desired moisture content, the designer will have to select the correct combination of inlet gas humidity, inlet gas temperature, and dryer residence time. In the case of hydrated salts that carry water of crystallization, high temperatures may be needed to drive off the final moisture.

The moisture content of the solid phase is usually expressed as mass of moisture per mass of bone-dry solids. The residual moisture remaining when the solids reach equilibrium with the entering gas is referred to as the equilibrium moisture content. When a wet solid is dried experimentally, a curve like that shown in Fig. 18.58 is obtained. The rate of drying initially increases during a warm-up period, marked A to B in the figure. A constant-rate period is then observed, shown as B to C, during which free moisture is evaporated from the solid surface. During this period there

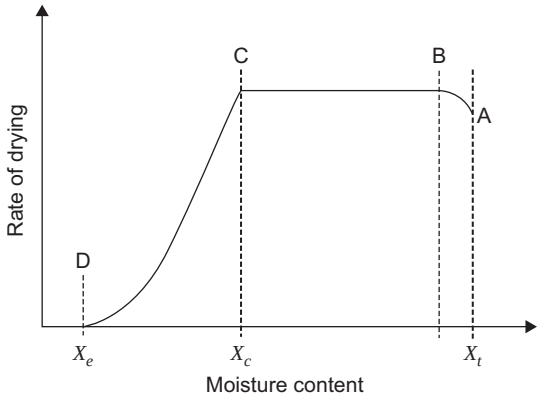


FIG. 18.58 Typical drying curve.

is no internal resistance to movement of moisture and the rate of evaporation is the same as that of a liquid of the same surface area. Once the free moisture is evaporated, the rate of drying starts to fall as internal mechanisms such as capillary drying and pore diffusion become more important, C to D. The falling-rate period is sometimes subdivided into regions dominated by different mechanisms.

The moisture content at the end of the constant-rate period is known as the critical moisture content, X_c. Moisture in excess of X_c is described as *free moisture*, and moisture removed between X_c and the equilibrium moisture content, X_e, is described as *bound moisture.* The critical moisture content can depend on the type of material, the particle size distribution, the type of dryer, and the thickness of solid layer (for tray and belt dryers). The critical moisture content increases with particle size and thickness of solids layer. The critical moisture content is easily determined experimentally in a drying test, but cannot reliably be predicted from theory. Some typical values of X_c are given in Green and Southard (2018) and range from 300% w/w for gelatin beads to 3% w/w for a 0.25-inch layer of sand on trays. Because the critical moisture content cannot be determined from first principles, estimation of dryer residence time must always be made experimentally, usually in plant trials carried out on an existing production line or in consultation with a dryer vendor.

Expressions for the rate of drying in the constant-rate period and falling-rate period are given in most textbooks on separations or mass transfer; see Chhabra and Gurappa (2019), McCabe et al. (2004), and Green and Southard (2018). During the constant-rate period the rate of drying is independent of the moisture content and depends only on the rates of heat and mass transfer. For a system that has only convective heat transfer:

$$-\frac{\mathrm{d}X}{\mathrm{d}t} = \frac{h\,A\,\Delta T}{\lambda} = K_G\,A(p_s - p_b) \tag{18.29}$$

where:

X = moisture content
t = time
h = heat transfer coefficient
A = gas–solids contact area
ΔT = temperature difference between the gas and solids, $= T_g - T_s$, where T_g is the temperature of the bulk gas and T_s is the temperature at the gas–liquid interface
λ = latent heat of vaporization
K_G = mass transfer coefficient
p_s = vapor pressure of liquid at the surface
p_b = vapor pressure of liquid in the bulk gas

By writing the vapor pressure of the liquid at the surface, p_s, as a function of the surface temperature, T_s, using an equation such as the Antoine equation, Equation 18.29 can be solved using the j-factor analogy to relate the heat and mass transfer coefficients, and hence the surface temperature during the constant-rate period can be found. This temperature will always be less than the boiling point of the liquid and corresponds to the wet bulb temperature of the gas. This does not give a good estimate of the solids outlet temperature, though, as the solids will heat up further during the falling-rate period and can approach the inlet gas temperature if the flow in the dryer is countercurrent.

Unfortunately, integration of Equation 18.29 to predict the residence time requires knowledge of the critical moisture content, X_c. The critical moisture content is also required to solve the equations for residence time in the falling-rate section. Because the experiments that measure X_c also yield the residence time, the theoretical analysis is somewhat superfluous and is generally only used when making modifications to an existing dryer.

An important consideration in dryer design is to properly match the solids and gas flows. The gas flow rate must be large enough to take up the moisture removed and to provide the necessary heat without requiring an excessively high inlet gas temperature. Depending on the dryer design, the gas velocity must also be chosen so as to prevent (or, if required, cause) fluidization or entrainment of the solids. The gas outlet condition depends on whether the gas flow is co-current, countercurrent, or cross-flow to the solids, but will generally be approaching equilibrium with the solids at the point where the gas exits the dryer.

The gas inlet temperature is often constrained by the maximum temperature to which the solids can be exposed. Thermally sensitive materials such as foods, pharmaceutical products, polymers, paper, and textiles can become charred or degraded if exposed to high temperatures. Operation with a lower inlet temperature will lead to a higher gas flow rate and may require a larger dryer.

The gas inlet moisture (or solvent) content depends on whether the gas is recirculated or predried; see Section 18.7.3. An initial estimate of the gas rate can be made from a simple heat balance:

$$m_s\ \lambda(X_i - X_o)\ \ +\ \ m_s\ C_{ps}\ (T_{si} - T_{so}) = (m_g + m_e)\ C_{pg}\ (T_i - T_o) \tag{18.30}$$

where:

m_s = mass flow of bone-dry solids
m_g = mass flow of dry gas
m_e = mass flow of solvent or water in entering gas
X_i = inlet moisture content
X_o = outlet moisture content
C_{ps} = specific heat capacity of solids
C_{pg} = specific heat capacity of gas
T_{si} = solids inlet temperature
T_{so} = solids outlet temperature
T_i = gas inlet temperature
T_o = gas outlet temperature
λ = latent heat of vaporization

The sensible heat change of the evaporated moisture is neglected in Equation 18.30, and the sensible heat change of the solids can also be neglected for an initial estimate. The designer should then confirm that the gas flow rate calculated is sufficient to provide a driving force for mass transfer at the outlet conditions:

$$\frac{(m_o/M_{wL})}{((m_g/M_{wG}) + (m_o/M_{wL}))} < \frac{p_s}{P} \tag{18.31}$$

where:

m_o = mass flow of moisture at the outlet = $m_e + m_s(X_i - X_o)$
M_{wG} = average molecular weight of the gas
M_{wL} = molecular weight of the liquid
P = pressure

Typically, a dryer will be designed for about 80% or 90% approach to equilibrium at the gas exit:

$$\frac{(m_o/M_{wL})}{((m_g/M_{wG}) + (m_o/M_{wL}))} \approx \frac{0.8p_s}{P} \tag{18.32}$$

Equations 18.30 and 18.32 can be solved together until satisfactory values of m_g, m_e, and T_i are obtained. These calculations can also be made using process simulation programs.

18.7.2 Selection and design of dryers

The main factors to be considered when selecting a dryer are:

1. Feed condition: solid, liquid, paste, powder, crystals
2. Feed concentration, the initial liquid content
3. Product specification: dryness required, physical form
4. Throughput required
5. Heat sensitivity of the product
6. Nature of the vapor: toxicity, flammability
7. Nature of the solid: flammability (dust explosion hazard), toxicity

The drying characteristics of the material can be investigated by laboratory and pilot plant tests, which are best carried out in consultation with the equipment vendors. Full descriptions of the various types of dryers and their applications are given in Green and Southard (2018), Mujumdar (2014), and Couper et al. (2012). Only brief descriptions of the principal types will be given in this section.

The basic types used in the chemical process industries are tray, band, rotary, fluidized, pneumatic, drum, and spray dryers. For removal of low amounts of moisture under diffusion-limited conditions, gravity dryers can also be considered. These consist of a silo with the solids in mass flow and a countercurrent flow of sweep gas; see Mehos (2009).

Tray dryers (Fig. 18.59)

Batch tray dryers are used for drying small quantities of solids and are used for a wide range of materials.

The material to be dried is placed in either solid bottomed trays over which hot air is blown or perforated bottom trays through which the air passes. If air passes through the trays, then the designer must ensure that the air velocity is not high enough to cause fluidization; see Section 18.2.2.

Batch dryers have high labor requirements, but close control can be maintained over the drying conditions and the product inventory, and they are suitable for drying fine powders and valuable products.

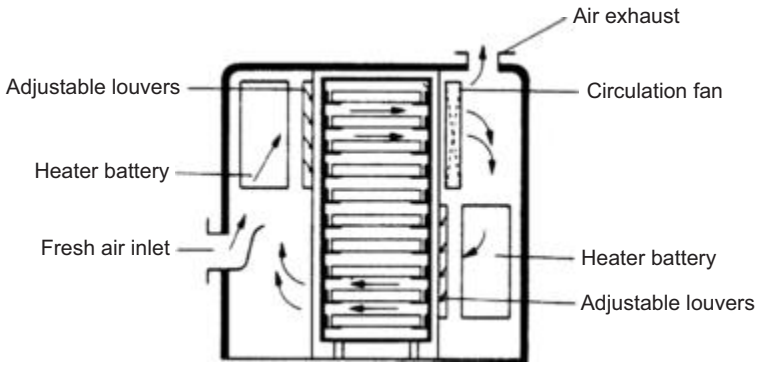


FIG. 18.59 Tray dryer.

Conveyor dryers (continuous circulation band dryers) (Fig. 18.60)

In this type, the solids are fed on to an endless, perforated conveyor belt. Hot air or other drying gas is either passed over the solids on the belt or forced through the belt. The belt is housed in a long rectangular cabinet, which is divided up into zones, so that the flow pattern and temperature of the drying air can be controlled. The relative movement through the dryer of the solids and drying air can be co-current, cross-flow, or, more usually, countercurrent.

This type of dryer is clearly only suitable for materials that form a bed with an open structure. High drying rates can be achieved with good product quality control. Thermal efficiencies are high, and with steam heating, steam usage can be as low as 1.5 kg per kg of water evaporated. The disadvantages of this type of dryer are high initial cost and, due to the mechanical belt, high maintenance costs. Care must be taken to ensure that the air velocity at dryer conditions is not high enough to cause fluidization of the bed if the flow is up through the belt.

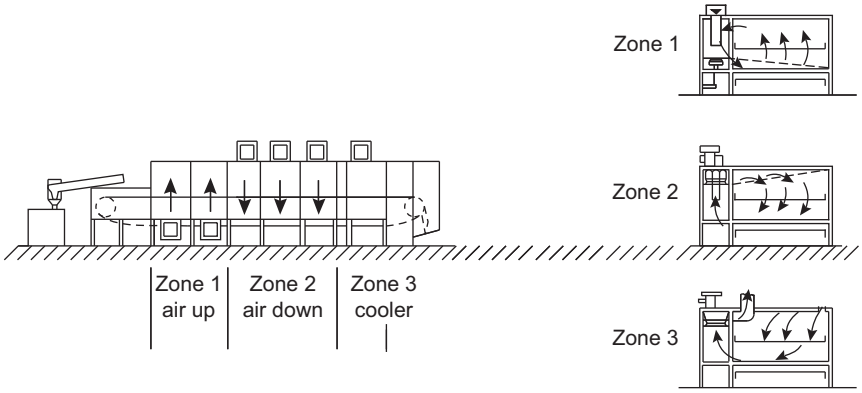


FIG. 18.60 Conveyor dryer.

Trays can also be used with belt dryers to allow continuous drying of fine powders. The trays are placed on the belt, filled with wet solids, passed through the dryer, emptied, and returned to the start. The trays can be fastened to the belt to eliminate manual retrieval.

Rotary dryer (Fig. 18.61)

In rotary dryers, the solids are conveyed along the inside of a rotating, inclined cylinder and are heated and dried by direct contact with hot air or gases flowing through the cylinder. In some, the cylinders are indirectly heated. Most commonly, the drying gas is heated by a steam heater at the dryer inlet or is direct-fired with a fuel.

Rotating dryers are suitable for drying free-flowing granular materials. They are suitable for continuous operation at high throughputs, have a high thermal efficiency, and have relatively low capital cost and labor costs. Some disadvantages of this type are nonuniform residence time, dust generation, and high noise levels. The superficial velocity of the gas in a rotary dryer should be low enough that the particles are not entrained in the gas flow; this sets the cylinder diameter if the gas rate is known. Rotary dryers can be quite large, and diameters over 15 ft are common, although 3 to 8 ft is the most typical size range. The main cost of a rotary dryer is usually the heater for the air, as the shell is not usually pressure-retaining and so is not a high-cost item. A cost correlation is given in Table 7.2 in terms of the heater surface area.

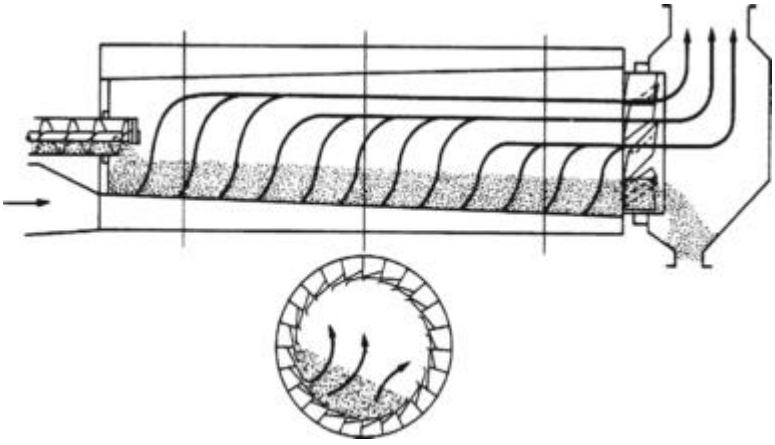


FIG. 18.61 Rotary dryer.

Fluidized-bed dryers (Fig. 18.62)

In this type of dryer, the drying gas is passed through the bed of solids at a velocity sufficient to keep the bed in a fluidized state, which promotes high heat transfer and drying rates.

Fluidized-bed dryers are suitable for granular and crystalline materials within the particle size range 0.5 to 3 mm. They are designed for continuous and batch operation.

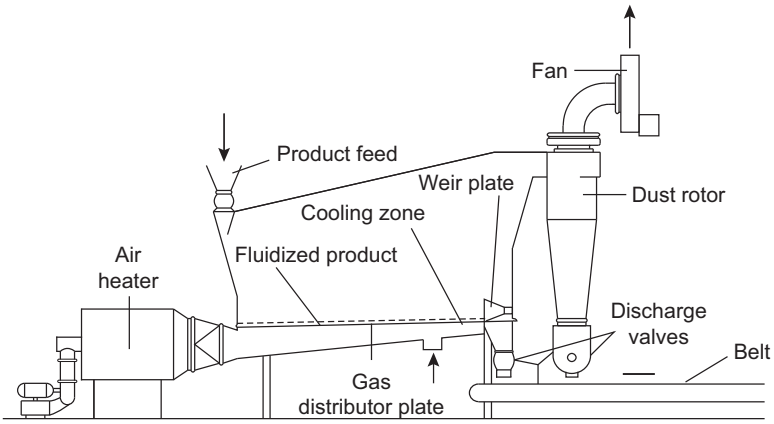


FIG. 18.62 Fluidized bed dryer.

The main advantages of fluidized dryers are rapid and uniform heat transfer; short drying times, with good control of the drying conditions; and low floor area requirements. The power requirements are high compared with other types.

A fluidized-bed dryer can be sized knowing the drying gas velocity and the superficial velocity required to cause fluidization; see Section 18.2.2. Cyclones are usually incorporated on the exit gas to prevent formation of dust from fine particles that are elutriated by the drying gas.

Pneumatic dryers (Fig. 18.63)

Pneumatic dryers, also called flash dryers, are similar in their operating principle to spray dryers. The product to be dried is dispersed into an upward-flowing stream of hot gas by a suitable feeder. The equipment acts as a

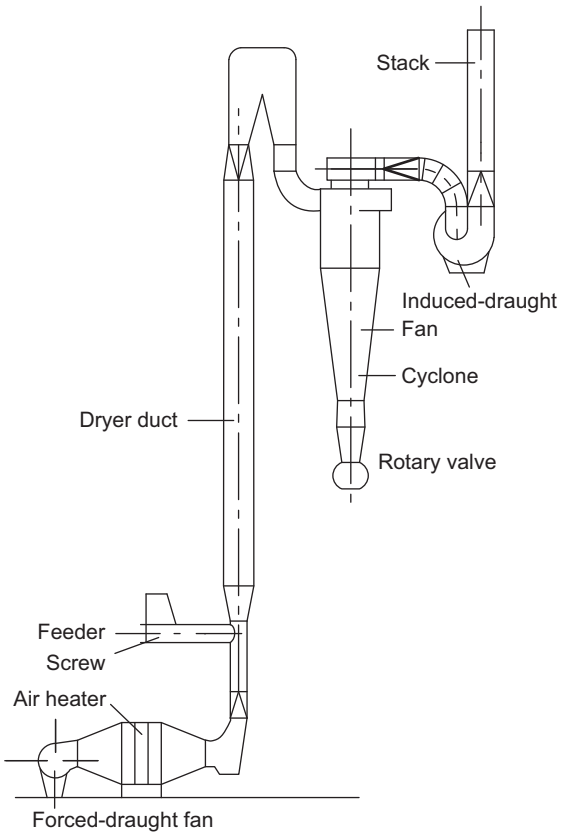


FIG. 18.63 Pneumatic dryer.

pneumatic conveyor and dryer. Contact times are short, and this limits the size of particle that can be dried. Pneumatic dryers are suitable for materials that are too fine to be dried in a fluidized-bed dryer but which are heat sensitive and must be dried rapidly. The thermal efficiency of this type is generally low.

Spray dryers (Fig. 18.64)

Spray dryers are normally used for liquid and dilute slurry feeds, but can be designed to handle any material that can be pumped. The material to be dried is atomized in a nozzle, or by a disc-type atomizer, positioned at the top of a vertical cylindrical vessel. Hot air flows up the vessel (in some designs downward) and conveys and dries the droplets. The liquid vaporizes rapidly from the droplet surface, and open, porous particles are formed. The dried particles are removed in a cyclone separator or bag filter.

The main advantages of spray drying are the short contact time, making it suitable for drying heat-sensitive materials, and good control of the product particle size, bulk density, and form. Because the solids concentration in the feed is low, the heating requirements will be high. Spray drying is discussed in the article by Møller and Fredsted (2009) and in a book by Masters (1991).

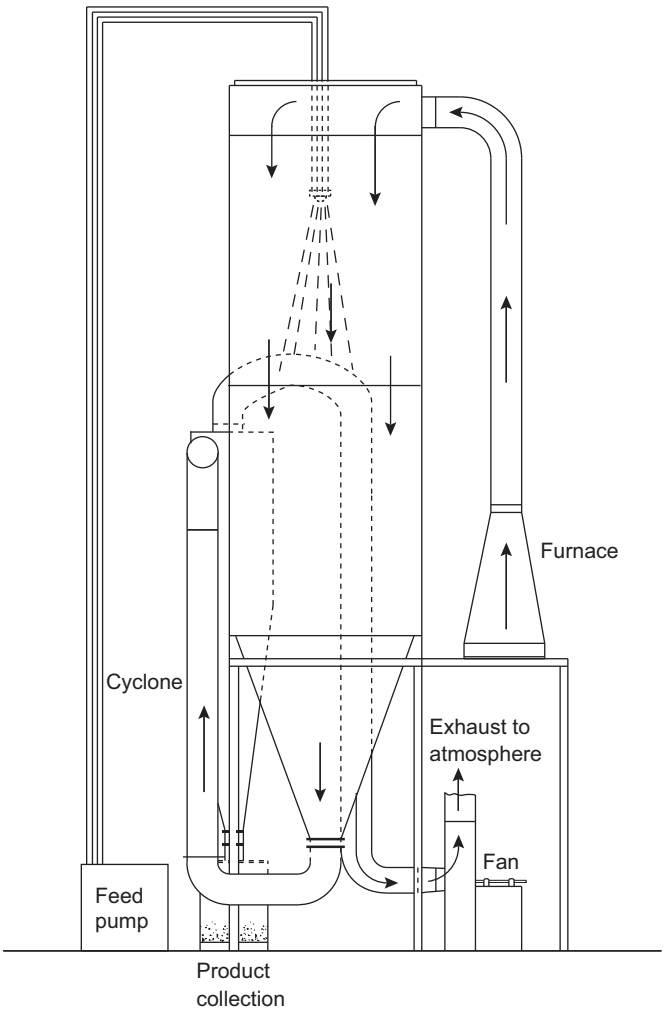


FIG. 18.64 Spray dryer.

Rotary drum dryers (Fig. 18.65)

Drum dryers are used for liquid and dilute slurry feeds. They are an alternative choice to spray dryers when the material to be dried will form a film on a heated surface and is not heat sensitive.

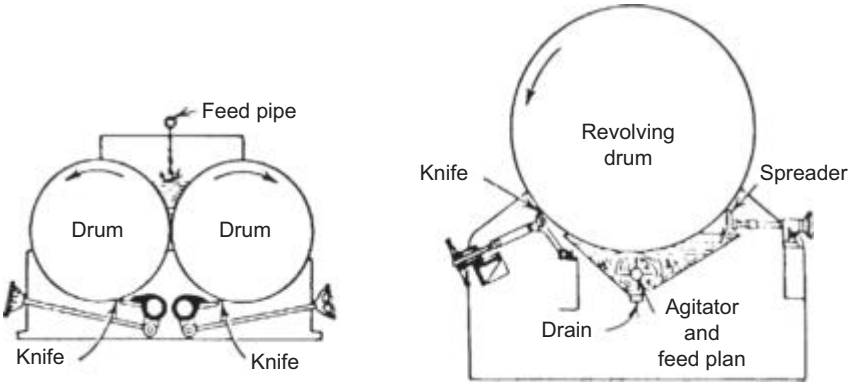


FIG. 18.65 Rotary drum dryers.

A drum dryer consists essentially of a revolving, internally heated drum, on which a film of the solids is deposited and dried. The film is formed either by immersing part of the drum in a trough of the liquid or by spraying, or splashing, the feed on to the drum surface; double drums are also used in which the feed is fed into the "nip" formed between the drums.

The drums are usually heated with steam, and steam economies of 1.3 kg steam per kg of water evaporated are typically achieved.

18.7.3 Process design and safety considerations

Dryers that remove water from solids usually use ambient air as the drying gas. The air can be heated in the dryer or pre-heated by indirect heat transfer from steam tubes at the dryer inlet. When high inlet temperatures are needed, direct heat transfer can be used by firing a burner in the inlet air. Such burners are typically fueled with natural gas or a process waste stream. The increase in inlet humidity due to the water vapor formed during combustion is not problematic if the inlet temperature is high.

For thermally sensitive products that must be dried with a low gas inlet temperature, the inlet air is sometimes preconditioned by passing it over a bed of molecular sieve adsorbent to ensure constant low inlet humidity. The adsorbent can then be regenerated in a temperature-swing cycle; see Section 16.2.1. Chilling the inlet air to remove moisture by condensation is also possible but is generally avoided, as chilling increases the heat load on the heater of the dryer.

The air or flue-gas flow exiting a once-through air—water dryer is usually ducted away from the dryer and discharged away from the plant. The exiting air will be hot and moist and may contain particulate material if the solids are prone to dust formation. Gas-cleaning systems will be specified if the dust load is high or if there are environmental or safety concerns with respect to the dust; see Section 18.5. The gas-cleaning equipment is usually located close to the dryer to prevent deposition of the dust or condensation in the ducting.

When a flammable solvent is removed from a solid or when a combustible dust could be formed, air should not be used as the drying gas. Although it is possible to design the dryer to operate outside the flammability envelope (see Section 10.2.2), there is nevertheless a risk that flammable conditions may occur during a process upset, with the potential to cause a fire or explosion. Instead, a closed-loop, recirculating gas system using an inert gas such as nitrogen can be used, as shown in Fig. 18.66.

In a closed-loop system, the gas leaving the dryer is sent to cyclones, filters, or other gas-cleaning equipment to remove dust. The cleaned gas is cooled to allow the solvent to be condensed and recovered. The gas is then compressed by a fan or blower and returned to the heater at the dryer inlet. The dryer in a closed-loop system is designed to be gas-tight, and a small amount of make-up gas may be added to allow for the gas that flows out in the void spaces of the solid product.

Recirculating gas dryers are also used when the solid has the potential to form a toxic or corrosive dust that would be harmful if discharged to the atmosphere. Note that not all dryers are suitable for operation in recirculating-gas mode. The dryer design must enable airtight operation.

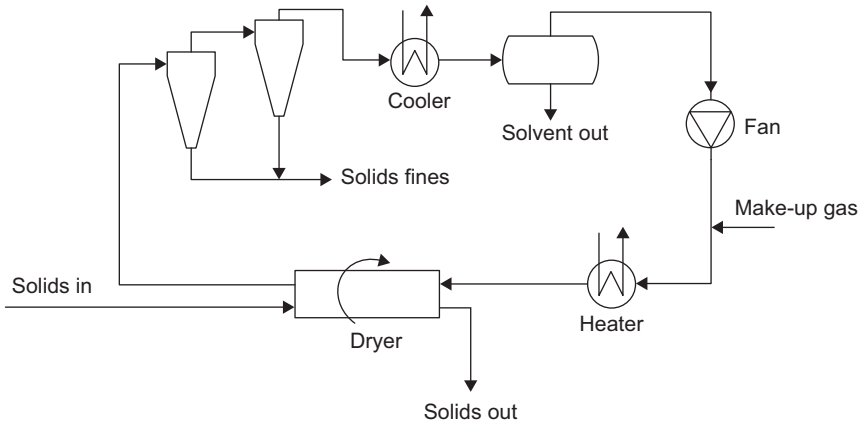


FIG. 18.66 Closed-loop drying process.

18.8 Solids formation, shaping, and size enlargement processes

Size enlargement processes are used to form larger agglomerates out of small particles. Size enlargement is a common step in processes that produce solid products, for example, in the manufacture of foods, tablets, fertilizers, catalysts, adsorbents, soap powders, solid fuels, and ceramics.

The equipment used for size enlargement is usually of proprietary design and must be specified in consultation with the vendor. The equipment vendors are easy to locate on the Web and usually have technically proficient sales engineers who can provide advice on device selection, dust handling, etc. In many cases, the vendor will be prepared to run demonstration trials to prove that their device forms an acceptable product.

There are several excellent specialist books on granulation and size enlargement: Pietsch (1991, 2005), Salman et al. (2006), and Lister and Ennis (2004). Useful introductions to the subject are also given in Green and Southard (2018), Rhodes (2008), Pietsch (1997), Higashitani et al. (2019), and Chhabra and Gurappa (2019).

18.8.1 Mechanisms of agglomeration

Agglomerates of smaller particles may be held together by natural cohesive forces between the particles or by partially melting the solids and sintering the particles together; however, in most cases a *binder* is added to the particles to stick them together. The choice of binder depends on the process temperature and product requirements. After the right size particles have been formed, the binder is sometimes driven off by drying or calcining the particles. Common binders for foods and pharmaceutical products include dextrose, starch, glucose, gelatine, and gums, whereas for catalysts or fertilizers, resins, clays, or water are usually used.

The theory of agglomeration processes is not well developed, and most size enlargement methods are difficult to model quantitatively. Instead, practitioners rely on experimentation and trial manufacturing runs to establish that the product will be formed with the desired density, strength, and other required properties. Scale-up experiments typically investigate varying the concentration and type of binder, as well as the process conditions, as it is often easier to achieve specifications by formulation changes than by changing process conditions, particularly if the product is to be made using existing equipment.

Four rate processes are important in forming an agglomerate out of smaller particles:

1. ***Wetting***: in which the binder contacts the surface of the powder.
2. ***Coalescence***: in which small particles adhere to one another to form a larger cluster.
3. ***Consolidation***: in which the clusters are compacted by forces transmitted to the cluster as a result of processing, for example, by collisions with other particles or with the vessel walls or agitator.
4. ***Breakage***: in which a weaker particle or shape is broken up due to collisions with other particles or the vessel.

Each of these processes can occur through several mechanisms. For example, breakage can occur by shattering of an agglomerate or abrasion of smaller particles from the surface.

The particle strength and shape depend on a trade-off between consolidation and breakage. High-shear devices that involve more particle−vessel and particle−particle collisions will tend to produce rounder, stronger pellets.

Particle density is obviously most affected by consolidation, which requires a high collision rate, but this must be traded off against breakage that would limit particle size. The different types of equipment used in forming solid particles are often designed to maximize the effectiveness of just one of these mechanisms. For example, tablet presses and roll presses strongly favor consolidation and seek to minimize breakage.

An overview of agglomeration mechanisms is given by Ennis (2010). The kinetics of particle formation and growth are discussed in more depth in Pietsch (1991, 1997), Salman et al. (2006), Lister and Ennis (2004), and Green and Southard (2018).

18.8.2 Shaping, forming, and size enlargement processes

The selection of agglomeration process depends on the size, shape, and uniformity of particles required. Some applications require a very uniform product. For example, tablets must be a standard size and shape to ensure that each contains the correct dose of active pharmaceutical ingredient. Fig. 18.67 gives a guide to selection of forming process based on desired particle size, but other factors should also be taken into consideration, as described next. Details of the design, construction, and operation of these processes are given in specialized books referenced in each section and in the handbooks listed in the introduction to Section 18.8.

Tablet presses and roll presses

When a uniform size product is required, a pressure compaction method is used. Rotary tablet presses or roll presses allow uniform shape and size solids to be produced at high throughputs, up to roughly 10,000 tablets per minute for a tablet press and 100 metric tons per hour for a roll press. Roll presses give less uniform product than tablet presses but allow larger briquettes to be formed.

The particles that are formed in a tablet press or roll press are usually of high density. The particle size distribution is very narrow, and particles up to the order of a few centimeters dimension can be formed. A wide range of shapes can be formed, including classic pill-shaped, lozenge-shaped, and briquettes. Tablet presses can also form intricate shapes and can imprint text or diameter indentations that make it easier for patients to split pills.

Tablet presses are widely used in the pharmaceuticals industry and are also used for food supplements and manufacture of certain types of candy. Roll presses are used in many other food processing applications, as well as in pelletizing of animal feeds and formation of briquettes.

The design and operation of tablet presses in the pharmaceutical industry are described in books by Carstensen (1977, 1993), Hickey and Ganderton (2009), and Parikh (2009).

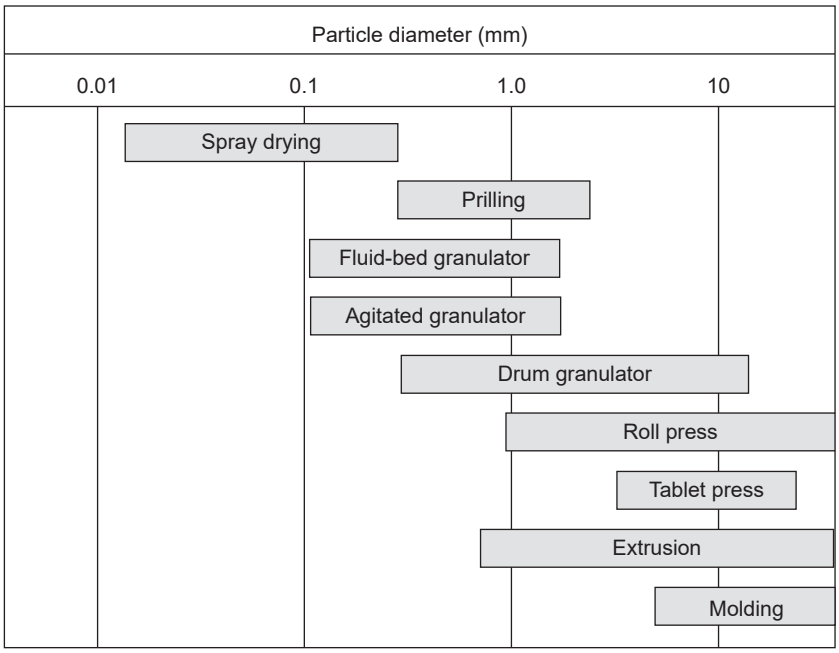


FIG. 18.67 Selection of particle-forming equipment.

Extrusion

An alternative form of pressure compaction is to form the solid and binder into a paste that can be extruded through a die. The resulting extrudate may either break up naturally, giving a product of uniform cross-section but varying length, or may be periodically cut with a knife edge or wire.

Extrusion can be used to form many different shapes of products, as evidenced by the many varieties of pasta, all of which are formed by this method. Extrudate particle cross-sectional diameter can range from less than a millimeter to a few centimeters. Extrusion processes are usually closely followed by dryers to ensure that the solids harden before they can stick together or lose their extruded shape. In addition to making pasta, some types of candy, and other formed food products, extrusion is often used for forming nonspherical catalysts. Extruded catalysts are usually formed as cylinders, but trilobes, tubes, and wagon wheel shapes are also used.

Spinning is a variant of extrusion that is used to form fibers. In polymer spinning, a melt, slurry, solution, or gel is extruded through a die known as a spinneret to form a fiber that can then be wound onto a bobbin. The spinneret usually contains several holes, allowing multiple filaments to be formed simultaneously. The fibers are often further processed by drawing (stretching) to achieve the desired fiber thickness. Spinning is used throughout the textile industry.

Molding

Mold presses can be used to accurately form large, complex shapes. Molding is used for making large, shaped ceramics and for forming shaped polymer objects. Molding processes usually incorporate a curing step, either by chemical or thermal treatment of the material inside the mold. For ceramics, this can be a high-temperature sintering, whereas for polymers, curing or cooling are used, depending on whether the polymer is thermosetting or thermoplastic. Polymers are usually melted and injected into the mold as a liquid (injection molding) to ensure full mold penetration.

Molding can allow highly accurate control of particle shape and dimensions. For large parts, additional machining may be used to remove burrs (flash) and add details. Molding is widely used in the manufacturing industries to make everything from automotive parts to toys and dinnerware.

Granulation

If a broader particle size distribution is acceptable, then particles can be agglomerated cheaply using a rotary agglomerator, also sometimes known as a granulator, pelletizer, tumbling drum, or balling drum. An agglomerator consists of an inclined drum into which the solids and binder are fed. Material leaving the drum is sent to a screen and undersize particles are recycled to the feed to act as seed particles (Fig. 18.68). Occasionally, oversize material is also separated, ground up, and returned to the feed. Inclined open pans can also be used as rotary agglomerators; these are cheaper, but produce more dust and require more recycle.

Larger size particles can also be formed in a granulation drum by spraying a slurry of small particles into the drum. The small particles coat the surface of the existing particles in the drum, causing larger particles to be formed. For crystalline materials, this method can be used to make large agglomerates containing many smaller crystalline particles.

The internally agitated mixers described in Section 18.4.11 can all be operated as granulators, with or without recycle of fines. If a binder is fed along with the solids, the solids will tend to agglomerate and form larger particles. Agitated granulators tend to form higher-density particles than drum granulators but operate at lower throughput.

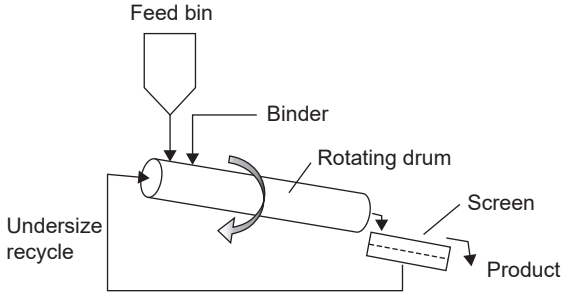


FIG. 18.68 Rotary agglomerator.

Large drum granulators are widely used in the manufacture of fertilizer pellets and can be designed for plant capacities up to the order of a thousand metric tons per hour. Granulation drums typically have 1- to 5-minute residence time, depending on the ease of agglomeration, and the solids holdup is usually between 10% and 20% of the internal volume. Smaller agitated granulators are used for making various bead products that must be approximately spherical and typically operate at a few metric tons per hour. These devices are often operated in batch mode. Some powdered foods are also made by granulation, for example, granulated sugar.

Fluidized beds can be used for granulation and also permit addition of a slurry of smaller particles. Care must be taken in a fluidized-bed granulator to ensure that the secondary feed is not elutriated before it can coat the particles of the bed. The design of fluidized beds is discussed in Section 18.2.2.

Spray drying and prilling

Spray drying was described in Section 18.7.2 and illustrated in Fig. 18.64. Prilling is essentially the same operation as spray drying but forms a larger particle, usually by crystallization combined with drying.

Spray drying and flash drying tend to form small, low-density particles. Particle sizes between ~10 and ~500 microns are typical. The particle shape can be quite variable and can range from spheres to flakes. Prilling forms larger particles, up to a few millimeters in diameter, and tends to form spheroids. The size of particles formed is strongly dependent on the spray nozzles used, and a wide range of proprietary designs are available from nozzle vendors. If a drying gas is used in countercurrent flow to the falling solids, then fines will be elutriated and must be collected from the effluent gas and recycled to the process.

Prilling is widely used for making fertilizers such as urea and ammonium nitrate. Spray drying is used to make catalysts, powdered foods, and detergent powders.

Crystallization

Crystallization can be used to form free-flowing solid particles from materials that will crystallize. Crystallization and precipitation are described in detail in Section 16.5, together with other processes for removing dissolved solids from a liquid.

18.8.3 Postforming processes

The first step after particle forming is usually to screen the particles to reject those that are undersized or oversized. Undersized material can usually be recycled to the forming step. Oversized material may need to be reground before it can be recycled.

Once the desired size and shape particles have been formed, they will often be dried or heat treated to reduce their plasticity and ensure that the shape is retained. In some cases, extreme heat treatment known as calcining will be carried out to drive off or burn off the binder.

Many solids products will subsequently be coated. Various types of coatings are applied; for example, pharmaceutical tablets may be coated with sugar or gels to make them more palatable or easier to swallow, while many solids are coated with waxes to suppress dust formation during handling. Coatings are usually applied in a tumbler or spray coating drum that is essentially the same as a rotary agglomerator. The particles must be kept moving during coating to ensure a uniform coating and prevent unwanted agglomeration. If the coating is applied in a solvent, then a rotary dryer is sometimes used as the coating drum. The selection of a coating material must consider the impact of the coating on the end-use application of the product.

18.9 Particle size reduction (comminution)

Crushing is the first step in the process of size reduction, reducing large lumps to manageable sized pieces. For some processes crushing is sufficient, but for chemical processes, it is usually followed by grinding to produce a fine-sized powder. Though many articles have been published on comminution, and Marshall (1974) mentions over 4000, the subject remains essentially empirical. The designer must rely on experience and the advice of the equipment manufacturers when selecting and sizing crushing and grinding equipment. The power requirements are best estimated based on grinding tests carried out on existing plant or in consultation with an equipment vendor. For a fuller treatment of the subject, the reader should refer to the books by Lowrison (1974), Prasher (1987), and Fuerstenau and Han (2003).

18.9.1 Crushing and grinding theory

Several models have been proposed for the calculation of the energy consumed in size reduction. None of these apply particularly well in practice, but they are suitable for making initial estimates of energy input for the purposes of undergraduate design projects. The energy required to overcome bonding forces in the solid and create new surface area is generally less than 1% of the energy consumed in a real mill, which is usually less than the error in closing an energy balance on the mill (Austin & Trass, 1997). For realistic estimates, the designer should always carry out trials in consultation with an equipment manufacturer.

Size reduction can occur through brittle fracture, shearing (cutting), and surface abrasion. The importance of different mechanisms depends on the material type and can also vary with particle size and temperature. For example, for rubber particles ground at low temperatures, brittle fracture will dominate, whereas at higher temperatures, the particles are more ductile and shearing is more important.

The most useful simple model of energy consumption is that developed by Bond (1952):

$$E = 100\, E_i \left(\frac{1}{\sqrt{d_2}} - \frac{1}{\sqrt{d_1}} \right) \tag{18.33}$$

where:

E = work done in grinding per unit mass feed (kWh/ton)
E_i = a constant known as the Bond work index (kWh/ton)
d_1 = initial particle size (m)
d_2 = final particle size (m)

The Bond work index is a constant and is equal to the amount of energy in kWh used to reduce a short ton (2000 lb) of solids from an initial theoretical infinite size to 80% passing 100 μm. In the original paper, Bond gave equations to adapt the work index for different types of equipment, but these equations have since become dated due to improvements in device and driver design. Work index values found in the literature should generally be treated with suspicion, as the device is often not specified, and the work index can vary substantially from one device to another. Average values of the work index can be misleading due to this device to device variation. Some average values of the Bond work index are given in Table 18.2, which can be used with Equation 18.33 for preliminary estimates of grinding work for the purposes of undergraduate design projects.

More sophisticated models of size reduction processes are usually formulated as population balance models that predict the rate of destruction and formation of particles in discretized size ranges. A breakage function can be used to predict the distribution of smaller particle sizes formed from grinding each particle size range. Rate of breakage functions can be determined experimentally in smaller mills and used to predict the required residence time and power to produce a desired particle size distribution from a given starting material in a larger mill. These models are usually proprietary.

18.9.2 Wet and dry grinding

In wet grinding, the solids are ground in a slurry, usually with the addition of surfactants known as grinding aids that modify the slurry viscosity and prevent the particles from agglomerating. Smaller particles can be formed in wet grinding than in dry grinding—sometimes as much as an order of magnitude smaller.

The work required in wet grinding is less than is needed in dry grinding for the same change in particle size. For wet grinding, the work index is typically about 75% of the work index for dry grinding.

Wet grinding causes substantially less dust formation than dry grinding. In some cases, use of gas cleaning equipment can be avoided, with resulting capital and operating cost savings.

Wet grinding tends to cause higher wear of the grinding equipment. The wet environment can cause corrosion of the grinding surfaces or grinding media, whereas abrasion by the solids prevents formation of a corrosion-resistant oxidized layer on the surface. Wet grinding equipment consequently requires more preventive maintenance.

The selection of wet or dry grinding is mainly determined by the downstream processing operations. If the solids are initially wet or if the liquid used for grinding is compatible with downstream process operations, then wet grinding is usually preferred. If surfactants or other additives are introduced, then these must also be compatible with downstream process operations.

18.9.3 Crushing and grinding (comminution) equipment

The main factors to be considered when selecting equipment for crushing and grinding are:

1. The size of the feed
2. The size reduction ratio
3. The required particle size distribution of the product
4. The throughput
5. The properties of the material: hardness, abrasiveness, stickiness, density, toxicity, flammability
6. Whether wet grinding is permissible

The selection guides given by Lowrison (1974) and Marshall (1974), which are reproduced in Fig. 18.69 and Table 18.14, can be used to make a preliminary selection based on particle size and material hardness. Detailed descriptions of most of the equipment listed in these tables are given in Chhabra and Gurappa (2019), Green and Southard (2018), Hiorns (1970), and Lowrison (1974); see also Austin and Trass (1997).

Crushing refers to coarse size reduction and is usually applied to large lumps of minerals entering a process. The most commonly used devices for coarse size reduction are jaw crushers and gyratory crushers. A jaw crusher crunches the material between a vertical fixed plate and a moving plate (Fig. 18.70a). A gyratory crusher is essentially a giant pestle and mortar in which the solids are crushed between an oscillating inner cone and a stationary outer cone (Fig. 18.70b). In both types of crusher, the size of the outlet opening determines the maximum particle dimension that is produced. If a finer particle size is required, then additional grinding machinery must be used downstream of the crusher. Sometimes two crushers will be used in series, with the downstream crusher having a narrower outlet to produce smaller particles.

Finer grinding is most often carried out in ball mills or their variants: pebble, rod, and tube mills. A ball mill is a cylindrical drum that contains a grinding medium such as metal balls. The drum is rotated and the feed material is crushed by impacts with the grinding medium. If flint, ceramic, or stone balls are used as a grinding medium, then it is referred to as a pebble mill, and if metal rods are used, then it is a *rod mill*. The diameter of the drum is usually less than the length, but for finer grinding a longer cylinder can be used, in which case the mill is called a tube mill. The grinding media are retained inside the drum by an inner screen, and feed and product are usually removed continuously. A schematic diagram of a typical ball mill is shown in Fig. 18.70(c). For very small particle sizes, a jet mill is used; see Liu (2017).

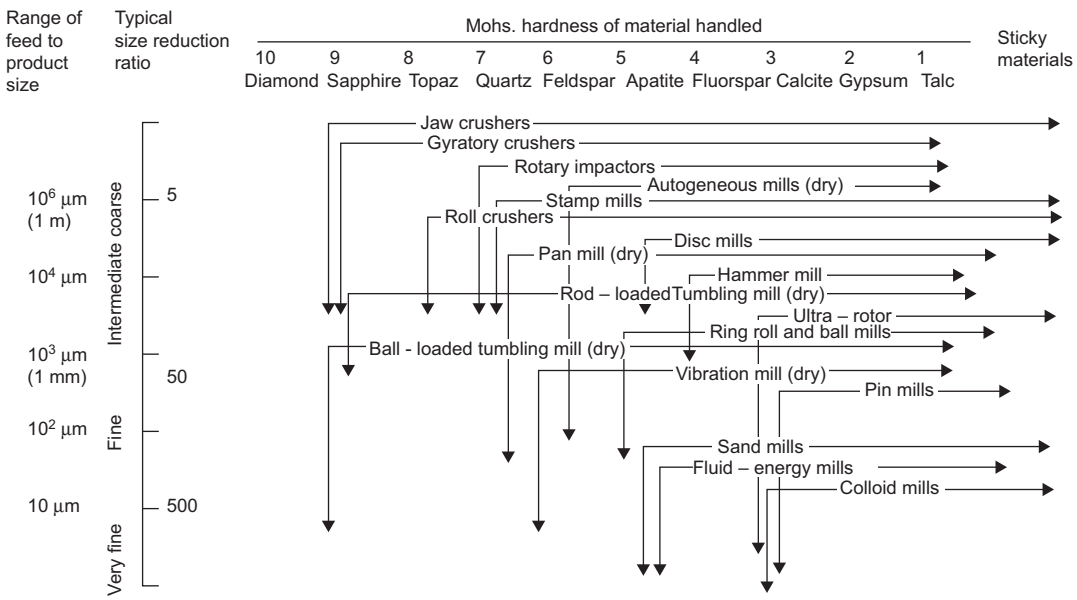


FIG. 18.69 Selection of comminution equipment. *(From Marshall, V. C. [1974]. Comminution. Institute of Chemical Engineers.)*

TABLE 18.14 Selection of comminution equipment for various materials

Material class no.	Material classification	Typical materials in class	Suitable equipment for product size classes			Remarks
			Down to 5 mesh	Between 5 and 300 mesh	Less than 300 mesh	
1	Hard and tough	Mica Scrap and powdered metals	Jaw crushers Gyratory crushers Cone crushers Autogeneous mills	Ball, pebble, rod and cone mills Tube mills Vibration mills	Ball, pebble and cone mills Tube mills Vibration and vibro-energy mills Fluid-energy mills	Mohs hardness 5—10, but includes other tough materials of lower hardness
2	Hard, abrasive and brittle	Coke, quartz, granite	Jaw crushers Gyratory and cone crushers Roll crushers	Ball, pebble, rod and cone mills Vibration mills Roller mills	Ball, pebble and cone mills Tube mills Vibration and vibro-energy mills Fluid-energy mills	Mohs hardness 5—10 High wear rate/ contamination in high-speed machinery Use machines with abrasion resistant linings
3	Intermediate hard, and friable	Barytes, fluorspar, limestone	Jaw crushers Gyratory crushers Roll crushers Edge runner mills Impact breakers Autogeneous mills Cone crushers	Ball, pebble, rod and cone mills Tube mills Ring roll mills Ring ball mills Roller mills Peg and disc mills Cage mills Impact breakers Vibration mills	Ball, pebble and cone mills Tube mills Perl mills Vibration and vibro-energy mills Fluid-energy mills	Mohs hardness 3—5
4	Fibrous, low abrasion and possibly tough	Wood, asbestos	Cone crushers Roll crushers Edge runner mills Autogeneous mills Impact breakers	Ball, pebble, rod and cone mills Tube mills Roller mills Peg and disc mills Cage mills Impact breakers Vibration mills Rotary cutters and dicers	Ball, pebble and cone mills Tube mills Sand mills Perl mills Vibration and vibro-energy mills cone mills	Wide range of hardness Low-temperature, liquid nitrogen, useful to embrittle soft but tough materials

5	Soft and friable	Sulfur, gypsum rock salt	Cone crushers Roll crushers Edge runner mills Impact breakers Autogeneous mills	Ball, pebble and cone mills Tube mills Ring roll mills Ring ball mills Roller mills Peg and disc mills Cage mills Impact breakers Vibration mills	Ball, pebble and cone mills Tube mills Sand mills Perl mills Vibration and vibro-energy mills Colloid mills Fluid-energy mills Peg and disc mills	Mohs hardness 1−3
6	Sticky	Clays, certain organic pigments	Roll crushers Impact breakers Edge runner mills	Ball, pebble, rod and cone mills* Tube mills* Peg and disc mills Cage mills Ring roll mills Colloid mills	Ball, pebble and cone mills* Tube mills* Sand mills Perl mills Vibration and vibro-energy mills	Wide range of Mohs hardness although mainly less than 3 Tends to clog *Wet grinding employed except for certain exceptional cases

Note: Moh's scale of hardness is given in Fig. 18.69.
** All ball, pebble, rod, and cone mills; edge runner mills; tube mills; vibration mills; and some ring ball mills may be used wet or dry except where stated. The perl mills, sand mills, and colloid mills may be used for wet milling only. From Marshall (1974).*

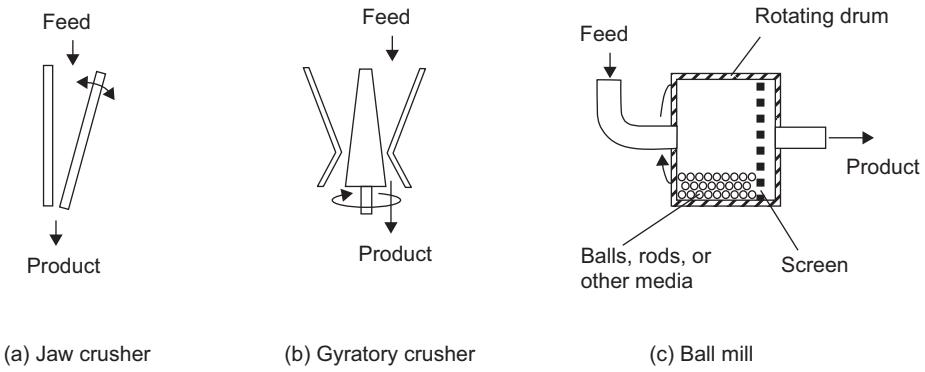


FIG. 18.70 Crushing and grinding equipment.

Ball mills are usually lined with a rubber liner to prevent wear of the casing. Abrasion or wear of the grinding media can be compensated by periodic continuous make-up of additional balls or by replacement of the media. Ball mills can be used in wet or dry grinding. The outer casing can be heated or cooled if necessary.

Ball mills are relatively inexpensive to install and operate. A preliminary estimate of the capital cost for a ball mill can be made using the equation given in Table 7.2.

18.9.4 Grinding cellular material

Grinding is often used as the initial step in recovery of biological products from cells. Grinding is used to break the cell walls so that components such as proteins can be extracted from the cell contents. Yeasts, molds, bacteria, algal, and mammalian cells have different grinding requirements because of differences in the cell wall strength and differences in the growth conditions.

The simplest method of cell disruption is to induce lysis (cell well breakage) by changing the osmotic potential of the solution, adding a surfactant that disrupts the cell wall or by adding an enzyme such as lysozyme, lysostaphin, or cellulase. These methods are widely used in small-scale preparations but can be difficult and expensive at commercial scale. For large-scale harvesting of cellular products, the cells are usually disrupted in a high-shear device known as a valve homogenizer or in a high-speed continuous bead mill. The beads are usually glass, ceramic, or steel balls, typically less than 1 mm in diameter. Enzymes or surfactants are often added to reduce the specific energy input and hence reduce potential product loss. Cooling of the mill may also be necessary to prevent thermal degradation of products.

The energy input required for grinding cellular material is difficult to predict from theory. Experiments or plant trials are usually carried out to optimize the extent of product recovery that can be obtained as a function of energy input and residence time.

18.9.5 Process design and safety considerations in crushing and grinding

Size reduction equipment is usually used in combination with particle classification equipment to achieve a desired particle size. The crushing or grinding equipment is followed by sieving or another classification process (see Section 18.4), with recycle of oversize material to the grinder. It is common to use two or more stages of grinding with intermediate recycles of oversize material when the goal is to produce a fine powder for further processing. The combination of a mill, classification process, and recycle is known as a mill circuit (Fig. 18.71).

Milling can cause considerable heating of the solids. If this reduces mill efficiency, it may be necessary to circulate the solids through a cooler or blow cooling air (or inert gas) through the grinder. If gas circulation is used, a gas cleaning system must be added to prevent emissions of particulate matter, as illustrated in Fig. 18.71.

Heating of the solids can be a significant hazard during comminution, particularly if the material is flammable or if dust formed by grinding can form an explosive mixture. When there is a concern about flammability or ignition, then grinding should be carried out in an inert atmosphere. The inert gas can be recycled through a cooler after the gas-cleaning step, if desired.

Wet grinding reduces the level of dust formation, but can also lead to hazards if the exposed surface of the solids is reactive with water or any other component of the grinding fluid.

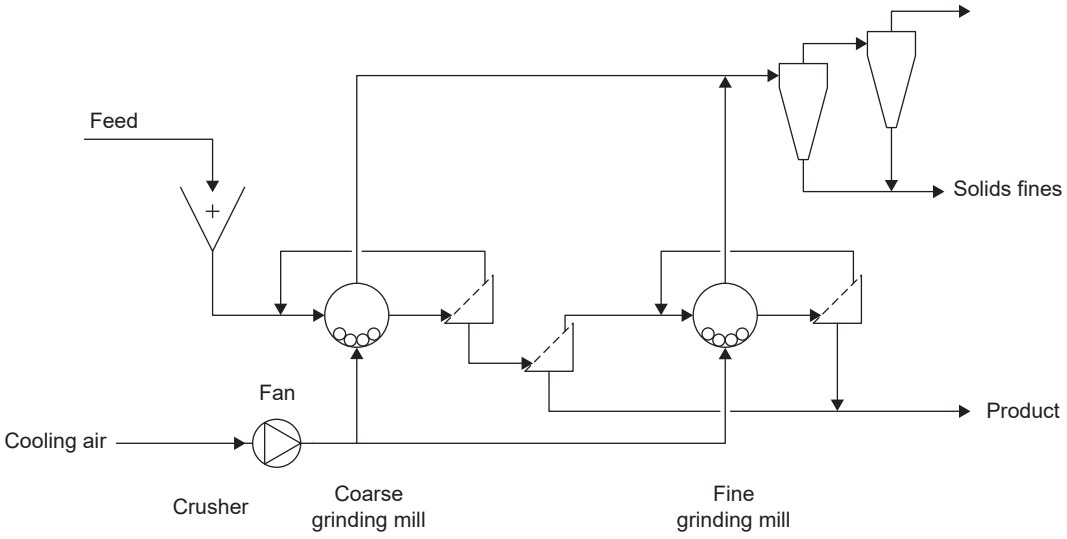


FIG. 18.71 Typical mill circuit.

Large crushers pose mechanical hazards in addition to the hazards listed earlier. With larger equipment it may be possible for workers to reach into or even fall into the machinery. Care should be taken to ensure that proper machine guarding is in place to prevent workers from entering the equipment. If blockages or jams occur, the equipment must be isolated and locked out from the power source before workers enter the equipment to clear the blockage.

Example 18.5

A coal gasification process is to be fed with 15 metric tons per hour of limestone to capture sulfur from the coal gas. The limestone is supplied with average dimension 1.5 cm and must be reduced to 20 mesh before feeding to the gasification process. Recommend equipment to achieve the desired particle size and estimate the work required.

Solution

From Table 18.1, 20 mesh corresponds to a sieve opening size of 0.85 mm. Assuming that the feed dimensions are on the same basis, the size reduction ratio is 15/0.85 = 17.6.

From Fig. 18.69, for a final particle size of ~1mm, with a Moh hardness of 4 (from Table 18.2), we could select a ball mill, rod mill, hammer mill, disc mill, or any of the crushers. In Table 18.14, limestone falls into material class 3, and for a product particle size range between 5 and 300 mesh, we would recommend a ball mill, rod mill, tube mill, roller mill, cage mill, impact breaker, or vibration mill. Because the size reduction ratio is not that large, it looks like a single-stage media mill such as a rod mill or ball mill will be adequate for this duty.

To make an estimate of the duty use Equation 18.33:

$$E = 100\, E_i \left(\frac{1}{\sqrt{d_2}} - \frac{1}{\sqrt{d_1}} \right) \tag{18.33}$$

From Table 18.2, E_i for limestone = 11.6, so:

$$E = 100 \times 11.6 \left(\frac{1}{\sqrt{0.00085}} - \frac{1}{\sqrt{0.015}} \right)$$

$$= 30.3 \times 10^3 \text{ kWh/ton}$$

1 short ton = 2000 lb and 1 metric ton = 2200 lb, so energy requirement = 1.1 × 30.3 = 33.3 MWh/metric ton.

A quick search on the Internet for rod mills can identify several devices that are suitable. For example, ESONG (a Chinese mining equipment supplier) makes a mill MBS2130 with diameter 2.1 m and length 3.6 m that can grind material <2.5 cm to a size range of 0.83 to 0.147 mm with capacity 14 to 35 metric tons/h and power consumption 155 kW. If this machine were operated for 1 hour and processed 15 metric tons of limestone, the specific power consumption would be 155 × 3600/15 = 37.2 MWh/metric ton, so the value from Equation 18.33 is not too bad an estimate. At this point the designer would

be ready to begin searching for vendors that had equipment that appeared to meet the specifications and could begin the process of qualifying vendors through test runs or reference cases.

18.10 Heat transfer to flowing solid particles

Particulate solids streams can have substantial heat capacity and hence significant heating or cooling requirements. It is often necessary to heat or cool a flowing solid stream at the entry or exit to a reactor or other process operation. When the heating or cooling requirement of the solids is small, the heat needed can be provided by additional heating or cooling of the fluid process streams that will contact the solids. When this is not feasible, a solids heater or cooler must be specified.

When the solids can be entrained in a liquid stream to form a slurry, then heat transfer can be carried out using conventional heat transfer equipment; see Chapter 19. Care must be taken to select exchanger designs that minimize dead spots where the slurry could settle and cause fouling. Slurries are usually fed on the tube side of shell and tube heat exchangers for this reason. The design must also allow for removal of the tube bundle or plates for cleaning.

Flowing solids in gas are usually heated or cooled by direct heat transfer with a hot or cold gas. Direct heat transfer can be accomplished in equipment similar to the continuous drying devices described in Section 18.7.2; the most common designs are the fluidized bed, rotary dryer, and flash dryer designs. Steam, flue gas from a burner, heated air, or heated process gases are used as heat sources, and cold air and nitrogen are the most commonly used coolants. Direct heat transfer between the gas and solid streams is very rapid in fluidized beds that have back-mixing of the solids. In other devices the heat transfer coefficient between the solids and fluid depends on the device geometry, flow pattern, and contact time. Few reliable correlations are available in the open literature, and the extent of heating or cooling achievable is best determined from plant trials or in consultation with an equipment vendor.

Direct heat transfer can also be accomplished by combustion of material dispersed on the solid surface. For example, in fluid catalytic cracking processes, the catalyst is heated by combustion of coke that forms as a by-product on the catalyst surface. Combustion of the coke regenerates the catalyst activity, as well as providing the heat needed for reaction and feed heating.

Indirect heat transfer to solids can be accomplished in any piece of solids handling equipment that can be fitted with a heating or cooling jacket or coil. The area available for heat transfer is generally low. If the solids are moving slowly, the heat transfer coefficient on the process side can be predicted from the correlations developed by Leva (1950) for heat transfer to packed or moving beds:

$$h = 0.813\frac{k}{D_T}e^{-6d_p/D_T}\left(\frac{d_pG}{\mu}\right)^{0.9} \quad \text{for}\frac{d_p}{D_T} < 0.35 \tag{18.34}$$

$$h = 0.125\frac{k}{D_T}\left(\frac{d_pG}{\mu}\right)^{0.75} \quad \text{for } 0.35 < \frac{d_p}{D_T} < 0.6 \tag{18.35}$$

where:

h = heat transfer coefficient
k = fluid thermal conductivity
d_p = particle diameter
D_t = vessel diameter
G = superficial mass velocity
μ = fluid viscosity

The heat transfer coefficient on the utility side can be found using the correlations for heat transfer to jacketed vessels given in Section 19.18.

Indirect heat transfer to or from a particulate solid flowing in a gas is less common and is usually accomplished by immersing heat transfer tubes into a fluidized bed of the solids. Heat transfer to and from fluidized beds has been the subject of much research, but there is significant variation in the measured data and consequently disagreement on

the best correlations to use. Heat transfer to and from fluidized beds is discussed in detail in Zenz and Othmer (1960). Green and Southard (2018) also give correlations for external walls, immersed tubes, and tube bundles.

18.11 Hazards of solids processing

In addition to the mechanical hazards inherent in solids-handling machinery, many solids-handling operations have the potential to form or release fine particulate material in the form of dust. Dust can pose a health hazard to workers who might inhale the dust, as well as creating the potential for dust explosions. Situations where dust can form are usually addressed at the design stage by the addition of engineering controls to mitigate dust formation and prevent the formation of toxic or explosive atmospheres.

18.11.1 Health impacts of dust inhalation

As a result of inadequate attention to worker safety in the early years of industrialization, the toxicological effects of worker exposure to many different types of dust have been well documented. Solids that have low inherent toxicity can nonetheless cause chronic health problems when absorbed into the bronchioles or alveoli as fine particulates. When dust reaches the lungs, it is absorbed by macrophages, which are subsequently swept out of the lungs by tiny hairs known as cilia. If the loading of dust is high or if the action of the cilia is impeded (for example, by lifestyle choices such as tobacco smoking), the macrophage system can be overwhelmed. Dead macrophages then accumulate in the lungs, releasing toxic substances that form scar tissue, leading to a condition known as *fibrosis*, in which the lungs lose their elasticity. Table 18.15 lists some of the chronic afflictions that have been traced to dust inhalation in different industries. These conditions are collectively known as *pneumoconiosis*, meaning "dusty lung." Health impacts of dust inhalation are discussed in more detail by Kaye (1997) and Baxter et al. (2010).

Whenever there are concerns over the toxicity or industrial hygiene impacts of dust formation, the designer should include appropriate engineering controls to reduce or eliminate worker exposure to dust. When feasible, use of wet process conditions will dramatically reduce dust formation. The primary engineering control on dust exposure is the plant itself. Plants that are susceptible to dust formation should be designed to operate under a slight vacuum so that dust cannot escape from the plant. A suction compressor is used to pull air from the plant and create a slight vacuum so that air flows into the equipment through any leaks but dust cannot flow out. Cyclones, filters, or other gas cleaning equipment are usually placed upstream of the suction compressor so that dust is not blown out to the environment; see Section 18.5. If it is not safe or feasible to pull air into the process (for example, if the dust is flammable), then the dust-forming equipment can be placed in a housing that is ventilated with an inert gas such as nitrogen.

A secondary control on dust formation is the building in which the plant is housed. Adequate ventilation should be provided to maintain dust concentrations below the limits required by health and safety legislation. Equipment should be cleaned regularly to prevent accumulations of dust, and cleaning should be carried out by washing or using approved vacuum cleaners rather than using brushes or brooms that would resuspend the dust in air. Finally,

TABLE 18.15 Health hazards of dust inhalation

Health problem	Cause (dust exposure)	Symptoms and effects
Asbestosis ("white lung")	Asbestos	Fibrosis, emphysema, mesothelioma (lung cancer)
Bagassosis	Moldy sugar cane	Fibrosis
Beryllium disease	Beryllium dust	Fibrosis
"Black lung" (coal pneumoconiosis)	Coal dust	Fibrosis, emphysema, lung cancer
"Brown lung" (byssinosis)	Cotton dust	Fibrosis, bronchitis, emphysema
"Farmer's lung"	Moldy hay, straw, or grain	Asthma, fibrosis, histoplasmosis
Silicosis	Silica, quartz, sand	Fibrosis, emphysema

workers may need to wear respirators or breathing masks when working around dust. The use of personal protective equipment, though often necessary, should never be viewed as a substitute for proper engineering design of the plant.

18.11.2 Dust explosions

If fine particles of a flammable material are suspended in air at the right concentration, an explosive mixture can be formed. If this mixture is ignited, the dust burns, releasing heat that can ignite more dust and hence propagate a flame front. The combustion of the dust leads to a large increase in molar volume and temperature and thereby creates a destructive pressure wave. Technically a dust explosion is usually a deflagration; however, if it occurs in a confined space such as inside a building, it can propagate into a detonation. Dust explosions that occur around solids-handling equipment also have the potential to disturb and suspend accumulated dust on or around the equipment, leading to secondary explosions that can be larger than the initial event.

Ignition sources for dust explosions can include hot equipment in grinders and driers, open flames, heat released by oxidation of exposed solid surfaces due to attrition or grinding, and electrostatic discharge sparks caused by the accumulation of static electricity on flowing powders.

During plant design, the design engineer should, whenever possible, seek conditions that minimize the likelihood of a dust explosion occurring. The design should avoid dust-forming operations, use wet processing when safe and feasible, eliminate ignition sources as much as possible, avoid dust accumulation, and make use of inert gas ventilation ("inerting"). The use of an inert sweep gas such as nitrogen in equipment that forms flammable dust is the most common method of explosion prevention, although some metal dusts will even react with nitrogen, in which case a noble gas such as argon must be used instead.

Dust explosion should be considered as a pressure relief scenario whenever flammable dusts are present. Methods for plant design to prevent or suppress explosions are discussed in more detail in Section 10.3.6 and in the National Fire Protection Association standards NFPA 61, NFPA 68, NFPA 69, NFPA 654, and NFPA 664. See also Mannan (2012), Field (1982), Cross and Farrer (1982), Grossel (1997), Barton (2001), Eckhoff (2003), and BS EN 1127.

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18.13 Nomenclature

		Dimensions in MLT
A	Gas−solids contact area in a dryer	$\mathbf{L}^2$
A_i	Area of interface	$\mathbf{L}^2$
A_{ps}	Projected area of a particle	$\mathbf{L}^2$
A_s	Surface area of cyclone	$\mathbf{L}^2$
A_1	Area of cyclone inlet duct	$\mathbf{L}^2$
C	Constant in Beverloo correlation (Equation 18.20)	—
C'	Constant in Nedderman version of the Beverloo correlation (Equation 18.21)	—
C_{ps}	Specific heat capacity of solids	$\mathbf{L}^2\mathbf{T}^{-2}\boldsymbol{\theta}^{-1}$
C_{pg}	Specific heat capacity of gas	$\mathbf{L}^2\mathbf{T}^{-2}\boldsymbol{\theta}^{-1}$
c	cohesion	$\mathbf{M}\mathbf{L}^{-1}\mathbf{T}^{-2}$
D	Vessel diameter	$\mathbf{L}$
D_c	Cyclone diameter	$\mathbf{L}$
D_{c1}	Diameter of standard cyclone	$\mathbf{L}$
D_{c2}	Diameter of proposed cyclone design	$\mathbf{L}$

Continued

		Dimensions in MLT
D_o	Diameter of the opening at the base of a vessel	**L**
D_T	Tank or vessel diameter	**L**
d	Particle diameter	**L**
d_a	Diameter of a circle with same projected area as a particle	**L**
$\overline{d_a}$	Arithmetic mean diameter	**L**
$\overline{d_g}$	Geometric mean diameter	**L**
d_h	Effective hydraulic diameter of a particle	**L**
d_i	Diameter of particle i	**L**
d_p	Particle "diameter"	**L**
d_{pr}	Diameter of a circle with the same perimeter as a particle	**L**
d_s	Diameter of solid particle removed in a centrifuge	**L**
d_{st}	Stokes diameter of a particle	**L**
$\overline{d_{vs}}$	Volume surface mean diameter	**L**
d_1	Initial particle size in grinding	**L**
d_1	Mean diameter of particles separated in cyclone under standard conditions	**L**
d_2	Final particle size in grinding	**L**
d_2	Mean diameter of particles separated in proposed cyclone design	**L**
d_{50}	Particle diameter for which cyclone is 50% efficient	**L**
E	Work done in grinding per unit mass feed	$\mathbf{L^2T^{-2}}$
E_i	Bond work index	$\mathbf{L^2T^{-2}}$
f_c	Friction factor for cyclones	—
G	Superficial mass velocity	$\mathbf{ML^{-2}T^{-1}}$
g	Gravitational acceleration	$\mathbf{LT^{-2}}$
H	Depth of solids in a bin or hopper	**L**
h	Heat transfer coefficient	$\mathbf{MT^{-3}\theta^{-1}}$
K_G	Mass transfer coefficient	$\mathbf{LT^{-1}}$
k	Fluid thermal conductivity	$\mathbf{MLT^{-3}\theta^{-1}}$
k	Shape parameter in Beverloo correlation (Equation 18.20)	—
L	Liquid volumetric flow rate to a hydrocyclone	$\mathbf{L^3T^{-1}}$
L	Particle length (longest dimension)	**L**
L_b	Length of a bed of solids	**L**
L_c	Conveying distance	**L**
M_{wG}	Average molecular weight of the gas	**M**
M_{wL}	Molecular weight of the liquid	**M**
m_e	Mass flow rate of solvent or water in entering gas	$\mathbf{MT^{-1}}$
m_g	Mass flow rate of dry gas	$\mathbf{MT^{-1}}$
m_o	Mass flow rate of moisture at the outlet of a dryer	$\mathbf{MT^{-1}}$
m_s	Mass flow rate of bone dry solids	$\mathbf{MT^{-1}}$
m	Mass flow rate of solids	$\mathbf{MT^{-1}}$
N	Number of particles in a sample	—
P	Pressure	$\mathbf{ML^{-1}T^{-2}}$
P_{ps}	Perimeter of a particle	**L**
ΔP	Pressure differential (pressure drop)	$\mathbf{ML^{-1}T^{-2}}$
p	Power consumption	$\mathbf{ML^2T^{-3}}$
p_s	Vapor pressure of liquid at the surface	$\mathbf{ML^{-1}T^{-2}}$
p_b	Vapor pressure of liquid in the bulk gas	$\mathbf{ML^{-1}T^{-2}}$
Q	Volumetric flow rate of liquid through a centrifuge	$\mathbf{L^3T^{-1}}$
Q_1	Standard flow rate in cyclone	$\mathbf{L^3T^{-1}}$
Q_2	Proposed flow rate in cyclone	$\mathbf{L^3T^{-1}}$
r_e	Radius of cyclone exit pipe	**L**

		Dimensions in MLT
r_t	Radius of circle to which center line of cyclone inlet duct is tangential	**L**
T	Temperature	**θ**
T_g	Temperature of the bulk gas	**θ**
T_i	Gas inlet temperature	**θ**
T_o	Gas outlet temperature	**θ**
T_s	Temperature at the gas-liquid interface	**θ**
T_{si}	Solids inlet temperature	**θ**
T_{so}	Solids outlet temperature	**θ**
ΔT	Temperature difference between the gas and solids	**θ**
t	Time	**T**
t	Particle thickness	**L**
U	Fluid superficial velocity	$\mathbf{LT}^{-1}$
U_{mf}	Fluid superficial velocity at minimum fluidization	$\mathbf{LT}^{-1}$
u_g	Terminal velocity of solid particles settling under gravity	$\mathbf{LT}^{-1}$
u_1	Velocity in cyclone inlet duct	$\mathbf{LT}^{-1}$
u_2	Velocity in cyclone exit duct	$\mathbf{LT}^{-1}$
W	Particle width	**L**
X	Moisture content	—
X_c	Critical moisture content during drying	—
X_e	Moisture content in equilibrium with gas entering a dryer	—
X_i	Inlet moisture content	—
X_o	Outlet moisture content	—
α	Angle of internal friction	—
α_w	Angle of wall friction	—
B	Angle of repose	—
ε	Bed void fraction	—
ε_{mf}	Void fraction at minimum fluidization	—
η	Separating efficiency of a centrifuge	—
η	Efficiency of a cyclone in separating any particle of diameter d	—
λ	latent heat of vaporization	$\mathbf{L}^2\mathbf{T}^{-2}$
μ	Liquid (or fluid) viscosity	$\mathbf{ML}^{-1}\mathbf{T}^{-1}$
μ_c	Viscosity of continuous phase	$\mathbf{ML}^{-1}\mathbf{T}^{-1}$
μ_1	Cyclone test fluid viscosity	$\mathbf{ML}^{-1}\mathbf{T}^{-1}$
μ_2	Viscosity of fluid in proposed cyclone design	$\mathbf{ML}^{-1}\mathbf{T}^{-1}$
ρ_b	Bulk density of particulate solids	$\mathbf{ML}^{-3}$
ρ_{bf}	Flowing bulk density of a particulate solid	$\mathbf{ML}^{-3}$
ρ_c	Density of the continuous phase	$\mathbf{ML}^{-3}$
ρ_d	Density of the dispersed phase	$\mathbf{ML}^{-3}$
ρ_f	Fluid density	$\mathbf{ML}^{-3}$
ρ_L	Liquid density	$\mathbf{ML}^{-3}$
ρ_p	Particle (piece) density of a solid	$\mathbf{ML}^{-3}$
ρ_s	Density of solid	$\mathbf{ML}^{-3}$
ρ_t	True density of a solid particle	$\mathbf{ML}^{-3}$
ρ_w	Wetted particle density	$\mathbf{ML}^{-3}$
Δ_ρ	Difference in density between solid and liquid	$\mathbf{ML}^{-3}$
$\Delta_{\rho 1}$	Density difference under standard conditions in standard cyclone	$\mathbf{ML}^{-3}$
$\Delta_{\rho 2}$	Density difference in proposed cyclone design	$\mathbf{ML}^{-3}$
Σ	Sigma value for centrifuges, defined by equation 10.6	$\mathbf{L}^2$
σ	Normal stress (applied load)	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
σ_w	Normal stress at the wall	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
τ	Shear stress	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$

Continued

		Dimensions in MLT
τ_w	Shear stress at the wall	$\mathbf{ML^{-1}T^{-2}}$
ϕ	Factor in Fig. 18.35	—
X	Internal pore volume fraction of a particle	—
Ψ	Parameter in Fig. 18.35	—
Ψ	Particle sphericity in Equation 18.4	—
Dimensionless numbers		
Ar	Archimedes number (defined in Equation 18.17)	—
Re	Reynolds number	—
$\mathbf{Re_{mf}}$	Reynolds number at minimum fluidization	—

18.14 Problems

18.1. Design a storage and feed system for the grinder introduced in Example 18.5. It is desired to control the mass flow rate to the gasification process to within ±5% of set point.

18.2. A proposed belt dryer design has a 2-m-wide belt that will hold a 50-mm-thick layer of solids. The solid particles have average diameter 3 mm and piece density 730 kg/m^3. Hot air at 150 °C is blown up through the dryer belt at a volumetric flow rate of 7200 m^3/h per m^2 of belt area. Will the bed of solids on the belt fluidize?

18.3. The product from a crystallizer is to be separated from the liquor using a centrifuge. The concentration of the crystals is 6.5% and the slurry feed rate to the centrifuge will be 5.0 m^3/h. The density of the liquor is 995 kg/m^3 and that of the crystals 1500 kg/m^3. The viscosity of the liquor is 0.7 mN m^{-2}s. The cut-off crystal size required is 5 μm.

Select a suitable type of centrifuge to use for this duty.

18.4. Dissolved solids in the tar from the bottom of a distillation column are precipitated by quenching the hot tar in oil. The solids are then separated from the oil and burnt. The density of the solids is 1100 kg/m^3. The density of the liquid phase after addition of the tar is 860 kg/m^3 and its viscosity at the temperature of the mixture is 1.7 mN m^{-2}s. The solid content of the oil and tar mixture is 10% and the flow rate of the liquid phase leaving the separator will be 1000 kg/h. The cut-off particle size required is 0.1 mm.

List the types of separators that could be considered for separating the solids from the liquid. Bearing in mind the nature of the process, what type of separator would you recommend for this duty?

18.5. The solids from a dilute slurry are to be separated using hydrocyclones. The density of the solids is 2900 kg/m^3 and the liquid is water. A recovery of 95% of particles greater than 100 μm is required. The minimum operating temperature will be 10 °C and the maximum 30 °C. Design a hydrocyclone system to handle 1200 liters/min of this slurry.

18.6. A fluidized bed is used in the production of aniline by the hydrogenation of nitrobenzene. Single-stage cyclones, followed by candle filters, are used to remove fines from the gases leaving the fluidized bed.

The reactor operates at a temperature of 270 °C and a pressure of 2.5 bara. The reactor diameter is 10 m. Hydrogen is used in large excess in the reaction, and for the purposes of this exercise the properties of the gas may be taken as those of hydrogen at the reactor conditions. The density of the catalyst particles is 1800 kg/m^3.

The estimated particle size distribution of the fines is:

Particle size, μm	50	40	30	20	10	5	2
Weight less than	100	70	40	20	10	5	2

A 70% recovery of the solids is required in the cyclones.

For a gas flow rate of 100,000 m^3/h at the reactor conditions, determine how many cyclones operating in parallel are needed and design a suitable cyclone. Estimate the size distribution of the particles entering the filters.

18.7. What dryer would you recommend to process each of the following streams:

1. A continuous stream of shaped (extruded) breakfast cereal with flow rate 50 kg/h bone-dry mass and initial moisture content 150 wt% moisture.
2. A 10-kg batch of an enzyme.
3. A continuous flow of 100 dry kg/min of granulated sugar that contains 20% moisture and must be reduced to <1% moisture.
4. A slurry of heat-sensitive crystals with flow rate of 10 kg/h of solids and 30 kg/h of water.

CHAPTER

19

Heat transfer equipment

KEY LEARNING OBJECTIVES

- How to specify and design a shell and tube heat exchanger
- How to design boilers, thermosiphon reboilers, and condensers
- How to design a plate heat exchanger
- How to design air coolers and fired heaters
- How to determine whether a reactor can be heated or cooled using a jacket or internal coil

19.1 Introduction

The transfer of heat to and from process fluids is an essential part of most chemical processes. The most commonly used type of heat transfer equipment is the shell and tube heat exchanger, the design of which is the main subject of this chapter.

The fundamentals of heat transfer theory are covered in Chhabra and Shankar (2017) and in many other textbooks: Holman (2009), Ozisik (1985), Rohsenow et al. (1998), Kreith and Manglik (2017), and Bergman et al. (2011).

Several useful books have been published on the design of heat-exchange equipment. These should be consulted for more details on the construction of equipment and design methods than can be given in this book. A selection of the more useful texts is listed in the bibliography at the end of this chapter. The compilation edited by Schlünder (1983)—see also the edition by Hewitt (2009)—is probably the most comprehensive work on heat exchanger design methods available in the open literature. The book by Saunders (1988) is recommended as a good source of information on heat exchanger design, especially for shell and tube exchangers.

As with distillation, work on the development of reliable design methods for heat exchangers has been dominated in recent years by commercial research organizations: Heat Transfer Research, Inc. (HTRI) in the United States and Heat Transfer and Fluid Flow Service (HTFS) in the United Kingdom. The HTFS program was developed by the United Kingdom Atomic Energy Authority and the National Physical Laboratory, but is now available from Aspen Technology, Inc., and as part of the Honeywell UniSim Design Suite; see Chapter 4, Table 4.1. Their proprietary methods are not available in the open literature. They will, however, be available to design engineers in the major operating and contracting companies, whose companies subscribe to these organizations.

The principal types of heat exchangers used in the process industries, which will be discussed in this chapter, are listed here:

1. Double-pipe exchanger: the simplest type, used for cooling and heating
2. Shell and tube exchangers: used for all applications
3. Plate and frame exchangers (plate heat exchangers): used for heating and cooling

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4. Plate-fin exchangers
5. Spiral heat exchangers
6. Air cooled: used for coolers and condensers
7. Direct contact: used for cooling and quenching
8. Fired heaters
9. Agitated vessels

The word "exchanger" really applies to all types of equipment in which heat is exchanged, but is often used specifically to denote equipment in which heat is exchanged between two process streams. Exchangers in which a process fluid is heated or cooled by a plant service stream are referred to as heaters or coolers, respectively. If the process stream is vaporized, the exchanger is called a vaporizer if the stream is essentially completely vaporized; a *reboiler* if associated with a distillation column; and an *evaporator* if used to concentrate a solution (see Chapter 16). The terms *fired exchanger* and *fired heater* are used for exchangers heated by combustion gases, such as boilers; other exchangers are referred to as unfired exchangers.

19.2 Basic design procedure and theory

The general equation for heat transfer across a surface is:

$$Q = UA\Delta T_m \tag{19.1}$$

where Q = heat transferred per unit time, W
U = the overall heat transfer coefficient, $W/m^{2\circ}C$
A = heat transfer area, m^2
ΔT_m = the mean temperature difference, the temperature driving force, °C

The prime objective in the design of an exchanger is to determine the surface area required for the specified duty (rate of heat transfer) using the temperature differences available.

The overall coefficient is the reciprocal of the overall resistance to heat transfer, which is the sum of several individual resistances. For heat exchange across a typical heat exchanger tube, the relationship between the overall coefficient and the individual coefficients, which are the reciprocals of the individual resistances, is given by:

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln\left(\frac{d_o}{d_i}\right)}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} \tag{19.2}$$

where U_o = the overall coefficient based on the outside area of the tube, $W/m^{2\circ}C$
h_o = outside fluid film coefficient, $W/m^{2\circ}C$
h_i = inside fluid film coefficient, $W/m^{2\circ}C$
h_{od} = outside dirt coefficient (fouling factor), $W/m^{2\circ}C$
h_{id} = inside dirt coefficient, $W/m^{2\circ}C$
k_w = thermal conductivity of the tube wall material, $W/m^{\circ}C$
d_i = tube inside diameter, m
d_o = tube outside diameter, m

The magnitude of the individual coefficients depends on the nature of the heat transfer process (conduction, convection, condensation, boiling, or radiation), on the physical properties of the fluids, on the fluid flow rates, and on the physical arrangement of the heat transfer surface. As the physical layout of the exchanger cannot be determined until the area is known, the design of an exchanger is, of necessity, a trial-and-error procedure. The steps in a typical design procedure are as follows:

1. Define the duty: heat transfer rate, fluid flow rates, and temperatures.
2. Collect the fluid physical properties required: density, viscosity, heat capacity, and thermal conductivity.
3. Decide on the type of exchanger to be used.
4. Select a trial value for the overall coefficient, U.
5. Calculate the mean temperature difference, ΔT_m.
6. Calculate the area required from Equation 19.1.
7. Decide the exchanger layout.

8. Calculate the individual coefficients.
9. Calculate the overall coefficient and compare with the trial value. If the calculated value differs significantly from the estimated value, substitute the calculated for the estimated value and return to step 6.
10. Calculate the exchanger pressure drop; if unsatisfactory, return to steps 7 or 4 or 3, in that order of preference.
11. Optimize the design: repeat steps 4 to 10, as necessary, to determine the cheapest exchanger that will satisfy the duty. Usually this will be the one with the smallest area that satisfies the pressure drop constraint.

Procedures for estimating the individual heat transfer coefficients and the exchanger pressure drops are given in this chapter.

19.2.1 Heat exchanger analysis: The effectiveness–NTU method

The *effectiveness–NTU* method is a procedure for evaluating the performance of heat exchangers, which has the advantage that it does not require the evaluation of the mean temperature differences. *NTU* stands for the number of transfer units and is analogous with the use of transfer units in mass transfer; see Chapter 17.

The principal use of this method is in the rating of an existing exchanger. It can be used to determine the performance of the exchanger when the heat transfer area and construction details are known. The method has an advantage over the use of the design procedure outlined earlier, as an unknown stream outlet temperature can be determined directly, without the need for iterative calculations. It makes use of plots of the exchanger *effectiveness* versus *NTU*. The effectiveness is the ratio of the actual rate of heat transfer to the maximum possible rate.

The *effectiveness–NTU* method will not be covered in this book, as it is more useful for rating than design. The method is covered in books by Bergman et al. (2011), Ozisik (1985), and Hewitt et al. (1994). The method is also covered by the Engineering Sciences Data Unit in their Design Guides 98003 to 98007 (1998). These guides give large clear plots of effectiveness versus NTU and are recommended for accurate work.

19.3 Overall heat transfer coefficient

Typical values of the overall heat transfer coefficient for various types of heat exchangers are given in Table 19.1. More extensive data can be found in the books by Green and Southard (2018), TEMA (2019), and Coker (2015).

Fig. 19.1, which is adapted from a similar nomograph given by Frank (1974), can be used to estimate the overall coefficient for tubular exchangers (shell and tube). The film coefficients given in Fig. 19.1 include an allowance for fouling.

The values given in Table 19.1 and Fig. 19.1 can be used for the preliminary sizing of equipment for process evaluation and as trial values for starting a detailed thermal design.

19.4 Fouling factors (dirt factors)

Most process and service fluids will foul the heat transfer surfaces in an exchanger to a greater or lesser extent. The deposited material will normally have a relatively low thermal conductivity and will reduce the overall coefficient. It is therefore necessary to oversize an exchanger to allow for the reduction in performance during operation. The effect of fouling is allowed for in design by including the inside and outside fouling coefficients in Equation 19.2. Fouling factors are usually quoted as heat transfer resistances rather than coefficients. They are difficult to predict and are usually based on past experience. Estimating fouling factors introduces a considerable uncertainty into exchanger design; the value assumed for the fouling factor can overwhelm the accuracy of the predicted values of the other coefficients. Fouling factors are often wrongly used as factors of safety in exchanger design. Some work on the prediction of fouling factors has been done by HTRI; see Taborek et al. (1972). Fouling is the subject of books by Bott (1990) and Garrett-Price (1985) and is also discussed by Zhu (2014).

Typical values for the fouling coefficients and factors for common process and service fluids are given in Table 19.2. These values are for shell and tube exchangers with plain (not finned) tubes. More extensive data on fouling factors are given in the TEMA standards (2019) and by Coker (2015).

The selection of the design fouling coefficient will often be an economic decision. The optimum design will be obtained by balancing the extra capital cost of a larger exchanger against the savings in operating cost obtained from the longer operating time between cleaning that the larger area will give. Duplicate exchangers should be

TABLE 19.1 Typical overall coefficients

Shell and tube exchangers		
Hot fluid	**Cold fluid**	***U* (W/m^2°C)**
Heat exchangers		
Water	Water	800–1500
Organic solvents	Organic solvents	100–300
Light oils	Light oils	100–400
Heavy oils	Heavy oils	50–300
Gases	Gases	10–50
Coolers		
Organic solvents	Water	250–750
Light oils	Water	350–900
Heavy oils	Water	60–300
Gases	Water	20–300
Organic solvents	Brine	150–500
Water	Brine	600–1200
Gases	Brine	15–250
Heaters		
Steam	Water	1500–4000
Steam	Organic solvents	500–1000
Steam	Light oils	300–900
Steam	Heavy oils	60–450
Steam	Gases	30–300
Dowtherm	Heavy oils	50–300
Dowtherm	Gases	20–200
Flue gases	Steam	30–100
Flue	Hydrocarbon vapors	30–100
Condensers		
Aqueous vapors	Water	1000–1500
Organic vapors	Water	700–1000
Organics (some noncondensables)	Water	500–700
Vacuum condensers	Water	200–500
Vaporizers		
Steam	Aqueous solutions	1000–1500
Steam	Light organics	900–1200
Steam	Heavy organics	600–900

Air-cooled exchangers	
Process fluid	
Water	300–450

TABLE 19.1 Typical overall coefficients—cont'd

Air-cooled exchangers	
Process fluid	
Light organics	300–700
Heavy organics	50–150
Gases, 5–10 bar	50–100
10–30 bar	100–300
Condensing hydrocarbons	300–600

Immersed coils		
Coil	**Pool**	
Natural circulation		
Steam	Dilute aqueous solutions	500–1000
Steam	Light oils	200–300
Steam	Heavy oils	70–150
Water	Aqueous solutions	200–500
Water	Light oils	100–150

Immersed coils		
Coil	**Pool**	***U*** **(W/m^2°C)**
Agitated		
Steam	Dilute aqueous solutions	800–1500
Steam	Light oils	300–500
Steam	Heavy oils	200–400
Water	Aqueous solutions	400–700
Water	Light oils	200–300

Jacketed vessels		
Jacket	**Vessel**	
Steam	Dilute aqueous solutions	500–700
Steam	Light organics	250–500
Water	Dilute aqueous solutions	200–500
Water	Light organics	200–300

Gasketed-plate exchangers		
Hot fluid	**Cold fluid**	
Light organic	Light organic	2500–5000
Light organic	Viscous organic	250–500

Continued

TABLE 19.1 Typical overall coefficients—cont'd

	Gasketed-plate exchangers	
Hot fluid	**Cold fluid**	
Viscous organic	Viscous organic	100–200
Light organic	Process water	2500–3500
Viscous organic	Process water	250–500
Light organic	Cooling water	2000–4500
Viscous organic	Cooling water	250–450
Condensing steam	Light organic	2500–3500
Condensing steam	Viscous organic	250–500
Process water	Process water	5000–7500
Process water	Cooling water	5000–7000
Dilute aqueous solutions	Cooling water	5000–7000
Condensing steam	Process water	3500–4500

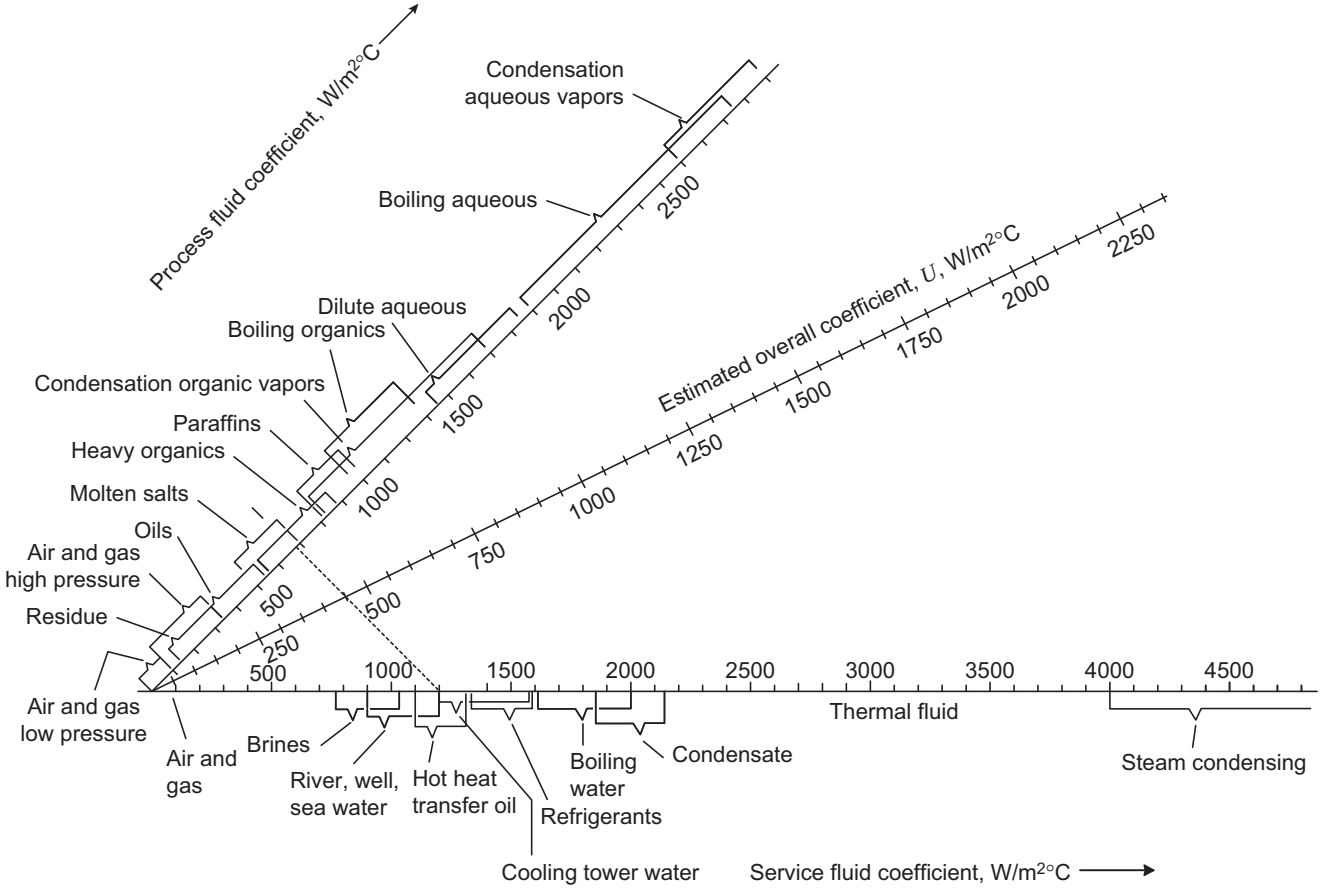


FIG. 19.1 Overall coefficients (join process side duty to service side and read *U* from center scale).

TABLE 19.2 Fouling factors (coefficients), typical values

Fluid	Coefficient (W/m^2°C)	Factor (resistance) (m^2°C/W)
River water	3000–12,000	0.0003–0.0001
Sea water	1000–3000	0.001–0.0003
Cooling water (towers)	3000–6000	0.0003–0.00017
Towns water (soft)	3000–5000	0.0003–0.0002
Towns water (hard)	1000–2000	0.001–0.0005
Steam condensate	1500–5000	0.00067–0.0002
Steam (oil free)	4000–10,000	0.0025–0.0001
Steam (oil traces)	2000–5000	0.0005–0.0002
Refrigerated brine	3000–5000	0.0003–0.0002
Air and industrial gases	5000–10,000	0.0002–0.0001
Flue gases	2000–5000	0.0005–0.0002
Organic vapors	5000	0.0002
Organic liquids	5000	0.0002
Light hydrocarbons	5000	0.0002
Heavy hydrocarbons	2000	0.0005
Boiling organics	2500	0.0004
Condensing organics	5000	0.0002
Heat transfer fluids	5000	0.0002
Aqueous salt solutions	3000–5000	0.0003–0.0002

considered for severely fouling systems so that one exchanger can be taken offline for cleaning while the plant continues to operate using the other exchanger.

When the design engineer adds area to allow for fouling, care must be taken to ensure that the velocity of the fluid is not reduced; otherwise, the fouling could be accelerated. For example, if more tubes are added to a shell and tube heat exchanger then the tube-side flow rate per tube is reduced. Lower tube-side velocity reduces the shear inside the tubes and increases the rate of tube-side fouling. An alternative method of increasing area would be to increase tube length, which comes at the expense of higher pressure drop.

19.5 Shell and tube exchangers: Construction details

The shell and tube exchanger is by far the most common type of heat transfer equipment used in the process industries. The advantages of this type are:

1. The configuration gives a large surface area in a small volume.
2. Good mechanical layout: a good shape for pressure operation.
3. Uses well-established fabrication techniques.
4. Can be constructed from a wide range of materials.
5. Easily cleaned.
6. Well-established design procedures.

Essentially, a shell and tube exchanger consists of a bundle of tubes enclosed in a cylindrical shell. The ends of the tubes are fitted into tubesheets, which separate the shell-side and tube-side fluids. Baffles are provided in the shell to direct the fluid flow and support the tubes. The assembly of baffles and tubes is held together by support rods and spacers (Fig. 19.2).

Exchanger types

The principal types of shell and tube exchangers are shown in Figs. 19.3 to 19.8. Diagrams of other types and full details of their construction can be found in the heat exchanger standards (see Section 19.5.1). The standard

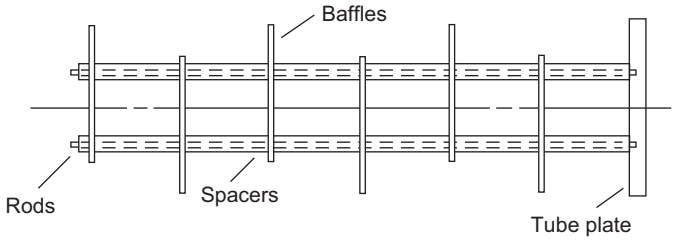


FIG. 19.2 Baffle spacers and tie rods.

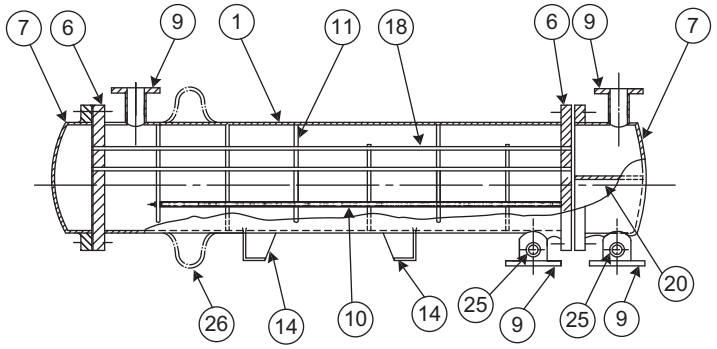


FIG. 19.3 Fixed-tube plate, type BEM. *Based on figures from BS 3274: 1960.*

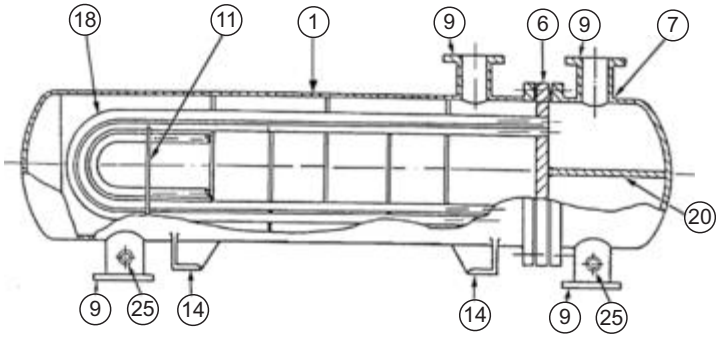


FIG. 19.4 U-tube, type BEU. *Based on figures from BS 3274: 1960.*

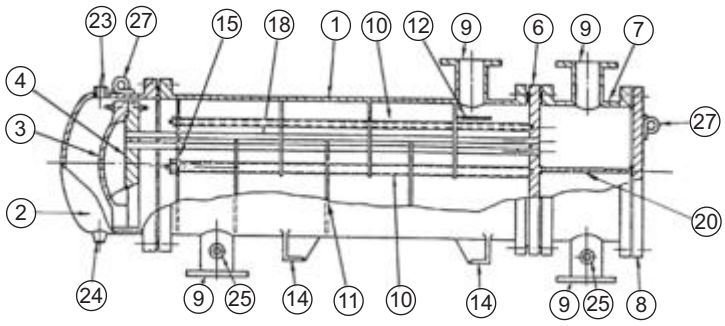


FIG. 19.5 Internal floating head without clamp ring, type AET. *Based on figures from BS 3274: 1960.*

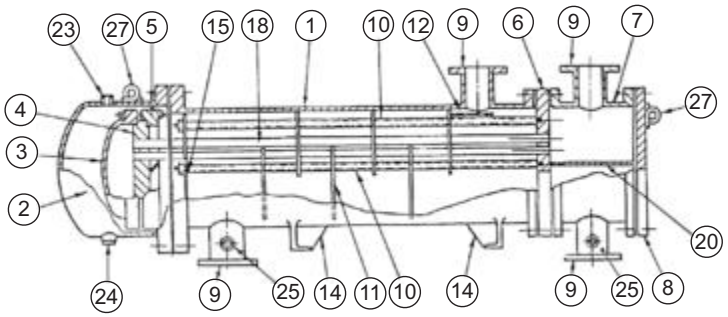


FIG. 19.6 Internal floating head with clamp ring, type AES. *Based on figures from BS 3274: 1960.*

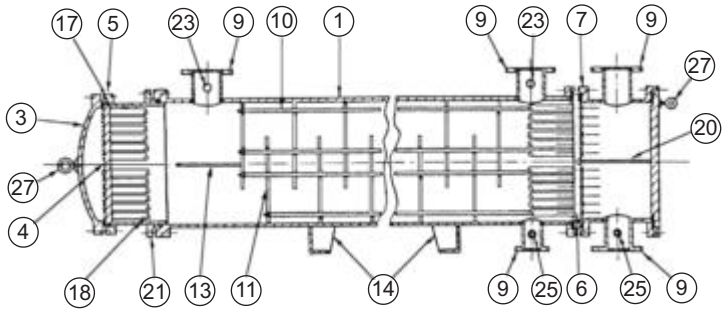


FIG. 19.7 External floating head, packed gland, type AEP. *Based on figures from BS 3274: 1960.*

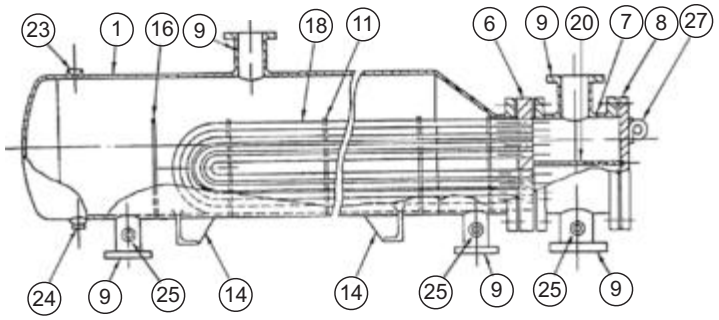


FIG. 19.8 Kettle reboiler with U-tube bundle, type AKU. *Based on figures from BS 3274: 1960.*

nomenclature used for shell and tube exchangers is given next; the numbers refer to the features shown in Figs. 19.3 to 19.8.

Nomenclature

Part number:

1. Shell
2. Shell cover
3. Floating-head cover
4. Floating-tube plate
5. Clamp ring
6. Fixed-tubesheet (tube plate)
7. Channel (end-box or header)

8. Channel cover
9. Branch (nozzle)
10. Tie rod and spacer
11. Cross baffle or tube-support plate
12. Impingement baffle
13. Longitudinal baffle
14. Support bracket
15. Floating-head support
16. Weir
17. Split ring
18. Tube
19. Tube bundle
20. Pass partition
21. Floating-head gland (packed gland)
22. Floating-head gland ring
23. Vent connection
24. Drain connection
25. Test connection
26. Expansion bellows
27. Lifting ring

The simplest and cheapest type of shell and tube exchanger is the fixed tubesheet design shown in Fig. 19.3 (TEMA type BEM). The main disadvantages of this type are that the tube bundle cannot be removed for cleaning and there is no provision for differential expansion of the shell and tubes. As the shell and tubes will be at different temperatures and may be of different materials, the differential expansion can be considerable, and the use of this type is limited to temperature differences up to about 80 °C. Some provision for expansion can be made by including an expansion loop in the shell (shown dotted on Fig. 19.3), but their use is limited to low shell pressure; up to about 8 bar. In the other types, only one end of the tubes is fixed and the bundle can expand freely.

The U-tube (U-bundle) type shown in Fig. 19.4 requires only one tubesheet and is cheaper than the floating-head types. This is the TEMA type BEU exchanger, which is widely used but is limited in use to relatively clean fluids, as the tubes and bundle are difficult to clean. It is also more difficult to replace a tube in this type.

Exchangers with an internal floating head (Figs. 19.5 and 19.6; TEMA types AET and AES) are more versatile than fixed-head and U-tube exchangers. They are suitable for high temperature differentials and, as the tubes can be rodded from end to end and the bundle removed, are easier to clean and can be used for fouling liquids. A disadvantage of the pull-through design (see Fig. 19.5) is that the clearance between the outermost tubes in the bundle and the shell must be made greater than in the fixed and U-tube designs to accommodate the floating-head flange, allowing fluid to bypass the tubes. The clamp ring (split flange design; see Fig. 19.6) is used to reduce the clearance needed. There will always be a danger of leakage occurring from the internal flanges in these floating-head designs.

In the external floating-head designs (Fig. 19.7; TEMA type AEP), the floating-head joint is located outside the shell and the shell sealed with a sliding gland joint employing a stuffing box. Because of the danger of leaks through the gland, the shell-side pressure in this type is usually limited to about 20 bar, and flammable or toxic materials should not be used on the shell side.

The kettle reboiler with U-tubes (TEMA type AKU) shown in Fig. 19.8 is commonly used for reboilers and evaporators that are heated with steam, as steam is a nonfouling service. TEMA type BKU without a removable channel cover is also widely used for kettle reboilers.

19.5.1 Heat exchanger standards and codes

The mechanical design features, fabrication, materials of construction, and testing of shell and tube exchangers are covered by the standards of the Tubular Heat Exchanger Manufacturers Association (TEMA). The TEMA standards cover three classes of exchangers: class R covers exchangers for the generally severe duties of the petroleum and related industries, class C covers exchangers for moderate duties in commercial and general process applications, and class B covers exchangers for use in the chemical process industries. The TEMA standards should be

consulted for full details of the mechanical design features of shell and tube exchangers; only brief details will be given in this chapter. Internationally, BS 3274 is also sometimes used, although the TEMA codes are most often followed.

The TEMA standards identify heat exchanger type by a three-letter code. The first letter denotes the tube-side head type, also known as the front end; the second letter identifies the shell type; and the third letter defines the rear end. Fig. 19.9 illustrates the TEMA nomenclature.

The standards give the preferred shell and tube dimensions; the design and manufacturing tolerances; corrosion allowances; and the recommended design stresses for materials of construction. The shell of an exchanger is a

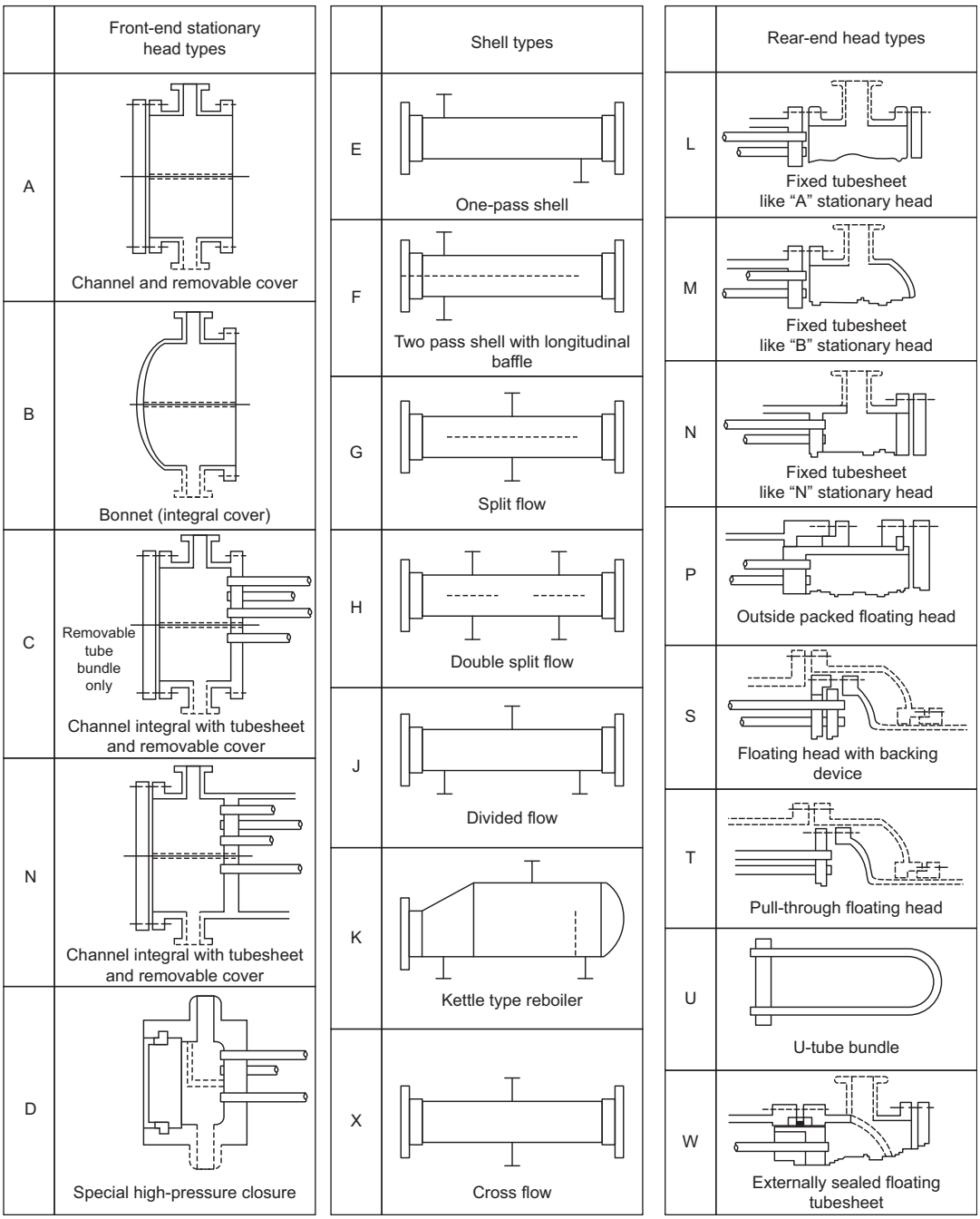


FIG. 19.9 TEMA designations for shell and tube heat exchangers. *Reproduced with permission from the Thermal Exchanger Manufacturers Association.*

pressure vessel and will be designed in accordance with the appropriate national pressure vessel code or standard; see Chapter 14, Section 14.2. The dimensions of standard flanges for use with heat exchangers are given in the TEMA standards.

In the TEMA standards dimensions are given in feet and inches, so these units have been used in this chapter with the equivalent values in SI units given in brackets.

19.5.2 Tubes

Dimensions

The TEMA design standard allows tube diameters between ¼ in. (6.4 mm) and 2 in. (50 mm), but tube diameters in the range ⅝ in. (16 mm) to 2 in. (50 mm) are most often used. The smaller diameters ⅝ to 1 in. (16 to 25 mm) are preferred for most duties, as they will give more compact, and therefore cheaper, exchangers. Larger tubes are easier to clean by mechanical methods and are selected for heavily fouling fluids.

The tube thickness (gauge) is selected to withstand the internal and external (shell-side) pressure and give an adequate corrosion allowance. TEMA standard tubing dimensions are given in table D-7 of the TEMA standards (D7-M in metric units), which is reproduced in *Perry's Chemical Engineers Handbook* (Green & Southard, 2018). The most commonly used thicknesses correspond to even-numbered Birmingham Wire Gauge (BWG) units. Standard diameters and wall thicknesses for steel tubes are given in Table 19.3.

The preferred lengths of tubes for heat exchangers are 6 ft. (1.83 m), 8 ft (2.44 m), 12 ft (3.66 m), 16 ft (4.88 m), 20 ft (6.10 m), and 24 ft (7.32 m). For a given surface area, the use of longer tubes will reduce the shell diameter. This will generally result in a lower-cost exchanger, particularly for high shell pressures, but will lead to an increase in pressure drop and pump work. The optimum tube length—to—shell diameter ratio will usually fall within the range of 5 to 10.

If U-tubes are used, the tubes on the outside of the bundle will be longer than those on the inside. The average length needs to be estimated for use in the thermal design. U-tubes will be bent from standard tube lengths and cut to size.

The tube size is often determined by the plant maintenance department standards, as clearly it is an advantage to reduce the number of sizes that have to be held in stores for tube replacement.

As a guide, ¾ in. (19 mm) is a good trial diameter with which to start design calculations.

Tube arrangements

The tubes in an exchanger are usually arranged in an equilateral triangular, square, or rotated square pattern (Fig. 19.10).

The triangular and rotated square patterns give higher heat transfer rates, but at the expense of a higher pressure drop than the square pattern. A square or rotated square arrangement is used for heavily fouling fluids, where it is necessary to mechanically clean the outside of the tubes. The recommended tube pitch (distance between tube centers) is 1.25 times the tube outside diameter; this will normally be used unless process requirements dictate otherwise. Where a square pattern is used for ease of cleaning, the recommended minimum clearance between the tubes is 0.25 in. (6.4 mm).

TABLE 19.3 Standard dimensions for steel tubes

Outside diameter (mm)	Wall thickness (mm)				
16	1.2	1.7	2.1	—	—
19	—	1.7	2.1	2.8	—
25	—	1.7	2.1	2.8	3.4
32	—	1.7	2.1	2.8	3.4
38	—	—	2.1	2.8	3.4
50	—	—	2.1	2.8	3.4

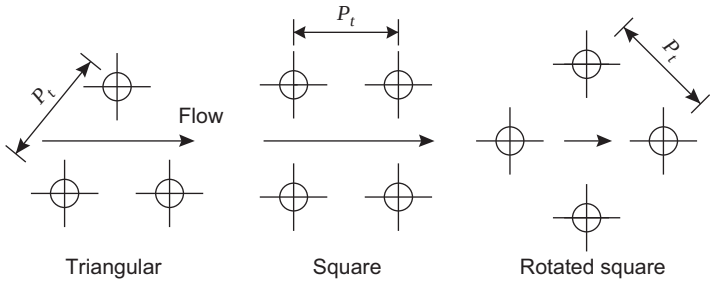


FIG. 19.10 Tube patterns.

Tube-side passes

The fluid in the tube is usually directed to flow back and forth in a number of "passes" through groups of tubes arranged in parallel to increase the length of the flow path. The number of passes is selected to give the required tube-side design velocity. Exchangers are built with from 1 to up to about 16 tube passes. The tubes are arranged into the number of passes required by dividing up the exchanger headers (channels) with partition plates (pass partitions). The arrangement of the pass partitions for two, four, and six tube passes are shown in Fig. 19.11. The layouts for higher numbers of passes are given by Saunders (1988).

19.5.3 Shells

The TEMA standards cover exchangers up to 60 in. (1520 mm) in diameter. Up to about 24 in. (610 mm), shells are normally constructed from standard, close tolerance pipe; above 24 in. (610 mm) they are rolled from plate.

For high-pressure applications, the shell thickness would be sized according to the pressure vessel design standards; see Chapter 14. The minimum allowable shell thickness is given in the TEMA standards. The values, converted to SI units and rounded, are given next.

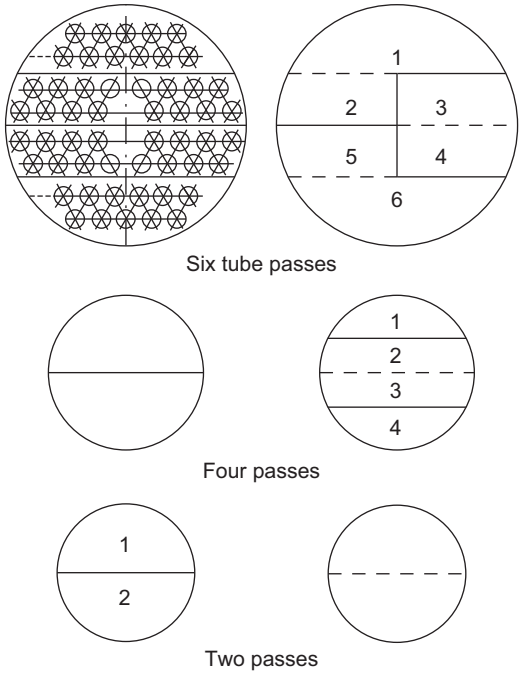


FIG. 19.11 Tube arrangements showing pass partitions in headers.

Minimum shell thickness (mm)

Nominal shell dia., mm	Carbon steel pipe	Alloy plate	Steel
150	7.1	—	3.2
200–300	9.3	—	3.2
330–580	9.5	7.9	3.2
610–740	—	7.9	4.8
760–990	—	9.5	6.4
1010–1520	—	11.1	6.4
1550–2030	—	12.7	7.9
2050–2540	—	12.7	9.5

The shell diameter must be selected to give as close a fit to the tube bundle as is practical to reduce bypassing around the outside of the bundle; see Section 19.9. The clearance required between the outermost tubes in the bundle and the shell inside diameter will depend on the type of exchanger and the manufacturing tolerances; typical values are given in Fig. 19.12.

19.5.4 Tubesheet layout (tube count)

The bundle diameter depends not only on the number of tubes but also on the number of tube passes, as spaces must be left in the pattern of tubes on the tubesheet to accommodate the pass partition plates.

An estimate of the bundle diameter D_b can be obtained from Equation 19.3b, which is an empirical equation based on standard tube layouts. The constants for use in this equation for triangular and square patterns are given in Table 19.4.

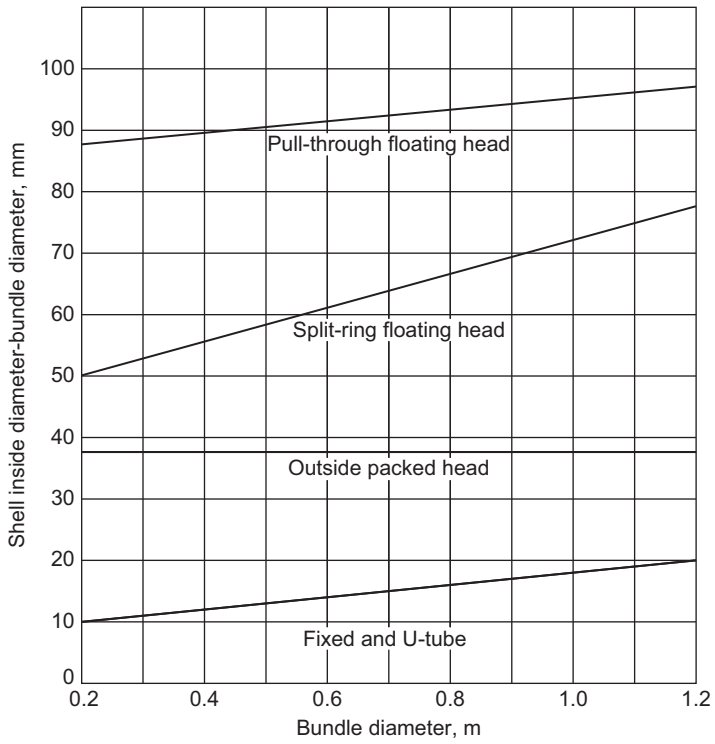


FIG. 19.12 Shell bundle clearance.

TABLE 19.4 Constants for use in Equation 19.3

Triangular pitch, $p_t = 1.25d_o$					
No. passes	**1**	**2**	**4**	**6**	**8**
K_1	0.319	0.249	0.175	0.0743	0.0365
n_1	2.142	2.207	2.285	2.499	2.675

Square pitch, $p_t = 1.25d_o$					
No. passes	**1**	**2**	**4**	**6**	**8**
K_1	0.215	0.156	0.158	0.0402	0.0331
n_1	2.207	2.291	2.263	2.617	2.643

$$N_t = K_1 \left(\frac{D_b}{d_o}\right)^{n_1}, \tag{19.3a}$$

$$D_b = d_o \left(\frac{N_t}{K_1}\right)^{1/n_1}, \tag{19.3b}$$

where N_t = number of tubes
D_b = bundle diameter, mm
d_o = tube outside diameter, mm

If U-tubes are used, the number of tubes will be slightly less than that given by Equation 19.3a, as the spacing between the two central rows will be determined by the minimum allowable radius for the U-bend. The minimum bend radius will depend on the tube diameter and wall thickness. It will range from 1.5 to 3.0 times the tube outside diameter. The tighter bend radius will lead to some thinning of the tube wall.

An estimate of the number of tubes in a U-tube exchanger (twice the actual number of U-tubes) can be made by reducing the number given by Equation 19.3a by one center row of tubes.

The number of tubes in the center row, the row at the shell equator, is given by:

$$\text{Tubes in center row} = \frac{D_b}{p_t}$$

where p_t = tube pitch, mm.

The tube layout for a particular design will normally be planned with the aid of computer programs. These will allow for the spacing of the pass partition plates and the position of the tie rods. Also, one or two rows of tubes may be omitted at the top and bottom of the bundle to increase the clearance and flow area opposite the inlet and outlet nozzles.

Tube count tables that give an estimate of the number of tubes that can be accommodated in standard shell sizes for commonly used tube sizes, pitches, and number of passes can be found in several books: Kern (1950), Coker (2015), Green and Southard (2018), and Saunders (1988).

Some typical tube arrangements are shown in Appendix H, available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

19.5.5 Shell types (passes)

The principal shell arrangements are shown in Fig. 19.9. The letters E, F, G, H, and J are those used in the TEMA standards to designate the various types. The E shell is the most commonly used arrangement.

Two shell passes (F shell) are occasionally used where the shell- and tube-side temperature differences are unsuitable for a single pass (see Section 19.6); however, it is difficult to obtain a satisfactory seal with a shell-side baffle, and the same flow arrangement can be achieved by using two shells in series.

The divided flow and split-flow arrangements (G and J shells) are used to reduce the shell-side pressure drop where pressure drop, rather than heat transfer, is the controlling factor in the design.

19.5.6 Shell and tube designation

A common method of describing an exchanger is to designate the number of shell and tube passes: m/n or $m{:}n$; where m is the number of shell passes and n the number of tube passes. So 1/2 or 1:2 describes an exchanger with one shell pass and two tube passes, and 2/4 an exchanger with two shell passes and four tube passes.

19.5.7 Baffles

Baffles are used in the shell to direct the fluid stream across the tubes to increase the fluid velocity and thus improve the rate of heat transfer. The most commonly used type of baffle is the single segmental baffle shown in Fig. 19.13(a); other types are shown in Fig. 19.13(b, c, and d).

Only the design of exchangers using single segmental baffles will be considered in this chapter.

If the arrangement shown in Fig. 19.13(a) were used with a horizontal condenser, the baffles would restrict the condensate flow. This problem can be overcome either by rotating the baffle arrangement through 90 degrees or by trimming the base of the baffle (Fig. 19.14).

The term *"baffle cut"* is used to specify the dimensions of a segmental baffle. The baffle cut is the height of the segment removed to form the baffle, expressed as a percentage of the baffle disc diameter. Baffle cuts from 15% to 45% are used. Generally, a baffle cut of 20% to 25% will be the optimum, giving good heat transfer rates without excessive pressure drop. There will be some leakage of fluid round the baffle, as a clearance must be allowed for assembly. The clearance needed depends on the shell diameter; typical values and tolerances are given in Table 19.5.

Another leakage path occurs through the clearance between the tube holes in the baffle and the tubes. The maximum design clearance will normally be $\frac{1}{32}$ in. (0.8 mm).

The minimum thickness to be used for baffles and support plates is given in the standards. The baffle spacings used range from 0.2 to 1.0 shell diameters. A close baffle spacing will give higher heat transfer coefficients, but at the expense of higher pressure drop. The optimum spacing will usually be between 0.3 and 0.5 times the shell diameter.

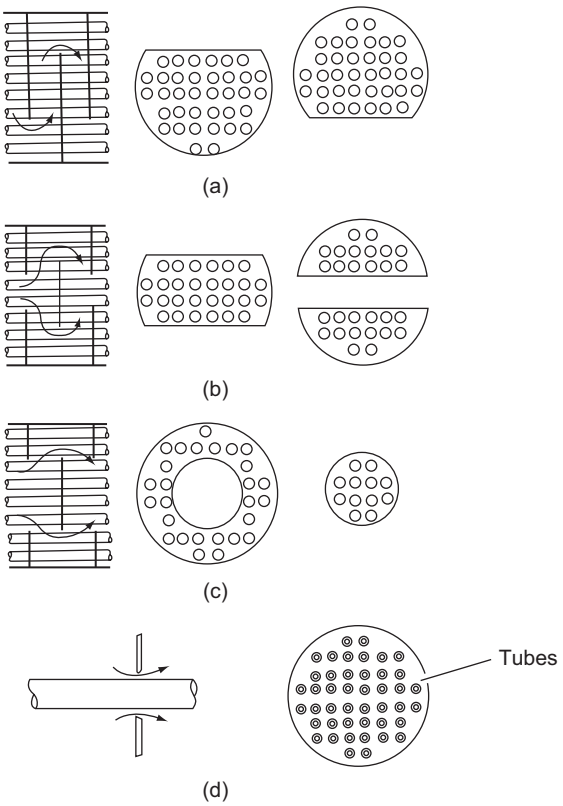


FIG. 19.13 Types of baffle used in shell and tube heat exchangers. (a) Segmental. (b) Segmental and strip. (c) Disc and doughnut. (d) Orifice.

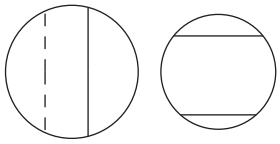


FIG. 19.14 Baffles for condensers.

TABLE 19.5 Typical baffle clearances and tolerances

Shell diameter, D_s	Baffle diameter	Tolerance
Pipe shells		
6–25 in. (152–635 mm)	$D_s - \frac{1}{16}$ in. (1.6 mm)	$+\frac{1}{32}$in. (0.8 mm)
Plate shells		
6–25 in. (152–635 mm)	$D_s - \frac{1}{8}$ in. (3.2 mm)	$+0, -\frac{1}{32}$ in. (0.8 mm)
27–42 in. (686–1067 mm)	$D_s - \frac{3}{16}$ in. (4.8 mm)	$+0, -\frac{1}{16}$ in. (1.6 mm)

19.5.8 Support plates and tie rods

Where segmental baffles are used, some will be fabricated with closer tolerances, 1⁄64 in. (0.4 mm), to act as support plates. For condensers and vaporizers, where baffles are not needed for heat transfer purposes, a few will be installed to support the tubes.

The minimum spacings to be used for support plates are given in the standards. The spacing ranges from around 1 m for 16-mm tubes to 2 m for 25-mm tubes.

The baffles and support plate are held together with tie rods and spacers. The number of rods required depends on the shell diameter and ranges from four 16-mm-diameter rods, for exchangers under 380 mm in diameter; to eight 12.5-mm rods, for exchangers of 1-m diameter. The recommended number for a particular diameter can be found in the standards.

19.5.9 Tubesheets (plates)

In operation, the tubesheets are subjected to the differential pressure between shell and tube sides. The design of tubesheets as pressure vessel components is covered by the ASME BPV Code. Design formulae for calculating tubesheet thicknesses are also given in the TEMA standards.

The joint between the tubes and tubesheet is normally made by expanding the tube by rolling with special tools (Fig. 19.15). Tube rolling is a skilled task; the tube must be expanded sufficiently to ensure a sound leakproof joint, but not overthinned, thereby weakening the tube. The tube holes are normally grooved (Fig. 19.16a) to lock the tubes more firmly in position and to prevent the joint from being loosened by the differential expansion of the shell and

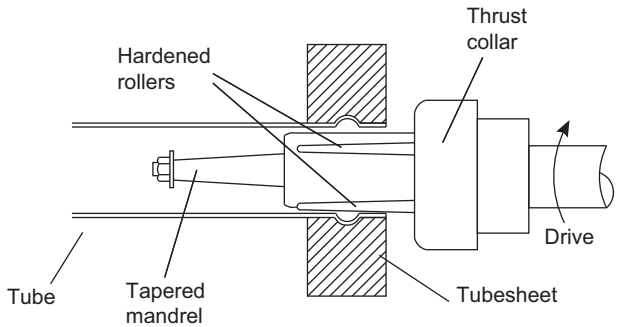


FIG. 19.15 Tube rolling.

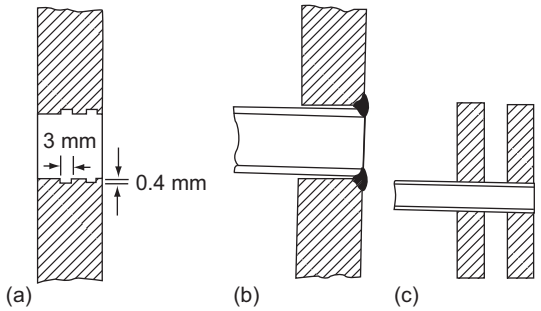


FIG. 19.16 Tube/tubesheet joints.

tubes. When it is essential to guarantee a leakproof joint, the tubes can be welded to the sheet (see Fig. 19.16b). This adds to the cost of the exchanger not only due to the cost of welding but also because a wider tube spacing is needed.

The tubesheet forms the barrier between the shell and tube fluids, and where it is essential for safety or process reasons to prevent any possibility of intermixing due to leakage at the tubesheet joint, double tubesheets can be used, with the space between the sheets vented (see Fig. 19.16c).

To allow sufficient thickness to seal the tubes, the tubesheet thickness should not be less than the tube outside diameter, up to about 25 mm diameter. Recommended minimum plate thicknesses are given in the standards.

The thickness of the tubesheet will reduce the effective length of the tube slightly, and this should be allowed for when calculating the area available for heat transfer. As a first approximation, the length of the tubes can be reduced by 25 mm for each tubesheet.

19.5.10 Shell and header nozzles (branches)

Standard pipe sizes are used for the inlet and outlet nozzles. It is important to avoid flow restrictions at the inlet and outlet nozzles to prevent excessive pressure drop and flow-induced vibration of the tubes. As well as omitting some tube rows (see Section 19.5.4), the baffle spacing is usually increased in the nozzle zone to increase the flow area. For vapors and gases, where the inlet velocities will be high, the nozzle may be flared, or special designs used, to reduce the inlet velocities (Fig. 19.17a and b). The extended shell design shown in Fig. 19.19(b) also serves as an impingement plate. Impingement plates are used when the shell-side fluid contains liquid drops or for high-velocity fluids containing abrasive particles.

19.5.11 Flow-induced tube vibrations

Premature failure of exchanger tubes can occur through vibrations induced by the shell-side fluid flow. Care must be taken in the mechanical design of large exchangers where the shell-side velocity is high, say greater than 3 m/s, to ensure that tubes are adequately supported.

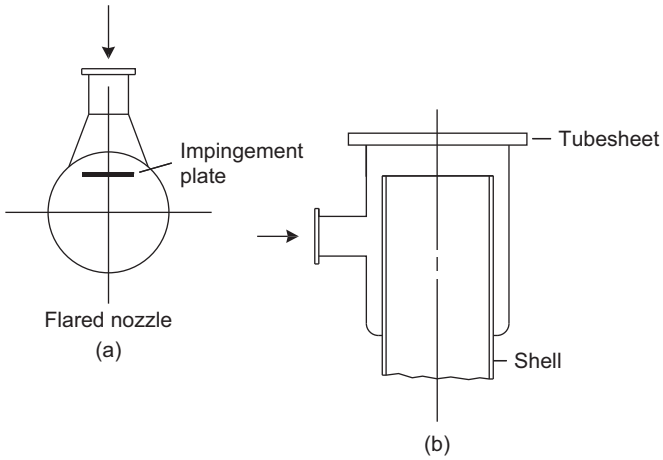


FIG. 19.17 Inlet nozzle designs.

The vibration induced by the fluid flowing over the tube bundle is caused principally by vortex shedding and turbulent buffeting. As fluid flows over a tube, vortices are shed from the downstream side, causing disturbances in the flow pattern and pressure distribution around the tube. Turbulent buffeting of tubes occurs at high flow rates due to the intense turbulence at high Reynolds numbers.

The buffeting caused by vortex shedding or by turbulent eddies in the flow stream will cause vibration, but large-amplitude vibrations will normally only occur above a certain critical flow velocity. Above this velocity, the interaction with the adjacent tubes can provide a feedback path that reinforces the vibrations. Resonance will also occur if the vibrations approach the natural vibration frequency of the unsupported tube length. Under these conditions, the magnitude of the vibrations can increase dramatically, leading to tube failure. Failure can occur either through the impact of one tube on another or through wear on the tube where it passes through the baffles.

For most exchanger designs, following the recommendations on support sheet spacing given in the standards will be sufficient to protect against premature tube failure from vibration. For large exchangers with high velocities on the shell side, the design should be analyzed to check for possible vibration problems. The computer-aided design programs for shell and tube exchanger design available from commercial organizations, such as HTFS and HTRI (see Section 19.1), include programs for vibration analysis.

Much work has been done on tube vibration over the past 20 years due to an increase in the failure of exchangers as larger sizes and higher flow rates have been used. Discussion of this work is beyond the scope of this book; for review of the methods used, see Saunders (1988) and Singh and Soler (1992). See also the Engineering Science Data Unit Design Guide ESDU 87019, which gives a clear explanation of mechanisms causing tube vibration in shell and tube heat exchangers and their prediction and prevention.

19.6 Mean temperature difference (temperature driving force)

Before Equation 19.1 can be used to determine the heat-transfer area required for a given duty, an estimate of the mean temperature difference, ΔT_m, must be made. This will normally be calculated from the terminal temperature differences: the difference in the fluid temperatures at the inlet and outlet of the exchanger. The well-known "logarithmic mean" temperature difference is only applicable to sensible heat transfer in true co-current or countercurrent flow, with linear temperature–enthalpy curves. This situation occurs when the heat capacities of both streams are constant and there is no phase change or if there is a phase change at constant pressure for a stream that contains a single component. These conditions are only approximated in reality. For countercurrent flow (Fig. 19.18a), the logarithmic mean temperature difference is given by:

$$\Delta T_{\text{lm}} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln \dfrac{(T_1 - t_2)}{(T_2 - t_1)}} \tag{19.4}$$

where ΔT_{lm} = log mean temperature difference
T_1 = hot fluid temperature, inlet
T_2 = hot fluid temperature, outlet
t_1 = cold fluid temperature, inlet
t_2 = cold fluid temperature, outlet

The equation is the same for co-current flow, but the terminal temperature differences will be $(T_1 - t_1)$ and $(T_2 - t_2)$. Strictly, Equation 19.4 will only apply when there is no change in the specific heats, the overall heat transfer coefficient is constant, and there are no heat losses. In design, these conditions can be assumed to be satisfied providing the temperature change in each fluid stream is not large.

In most shell and tube exchangers, the flow will be a mixture of co-current, countercurrent and, cross flow. Fig. 19.18(b and c) show typical temperature profiles for an exchanger with one shell pass and two tube passes (a 1:2 exchanger). Fig. 19.18(c) shows two different cases of temperature cross, where the outlet temperature of the cold stream is above that of the hot stream.

The usual practice in the design of shell and tube exchangers is to estimate the "true temperature difference" from the logarithmic mean temperature by applying a correction factor to allow for the departure from true countercurrent flow:

$$\Delta T_m = F_t \Delta T_{1\text{m}} \tag{19.5}$$

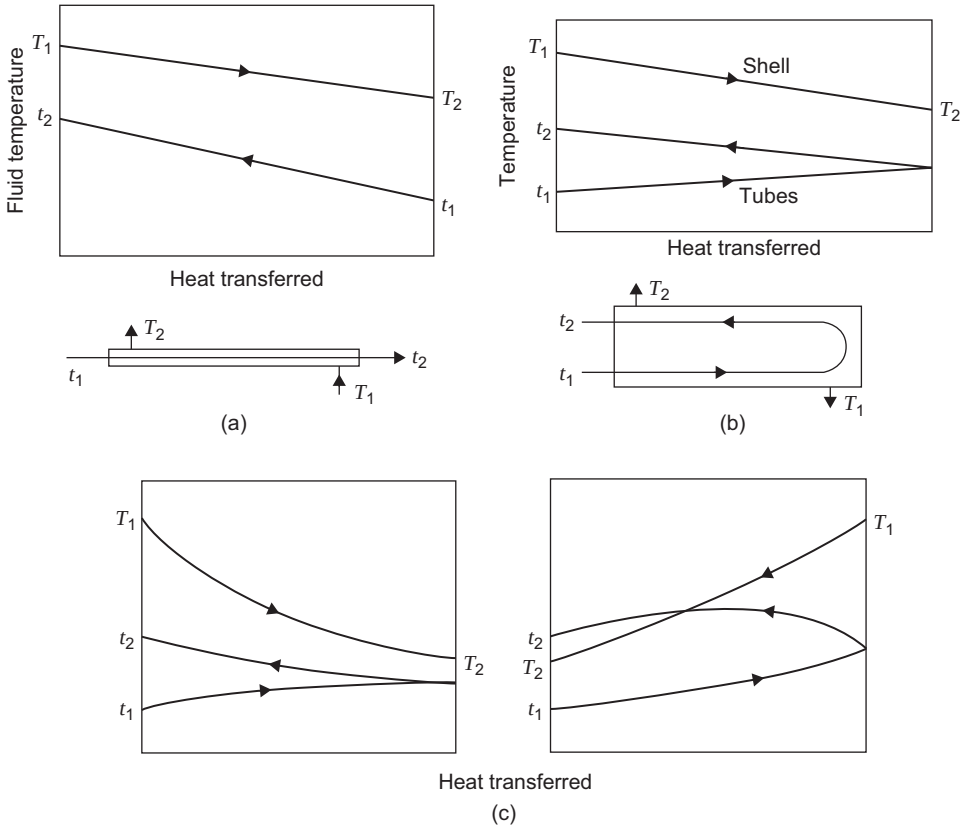


FIG. 19.18 Temperature profiles. (a) Countercurrent flow. (b) 1:2 exchanger. (c) Temperature cross.

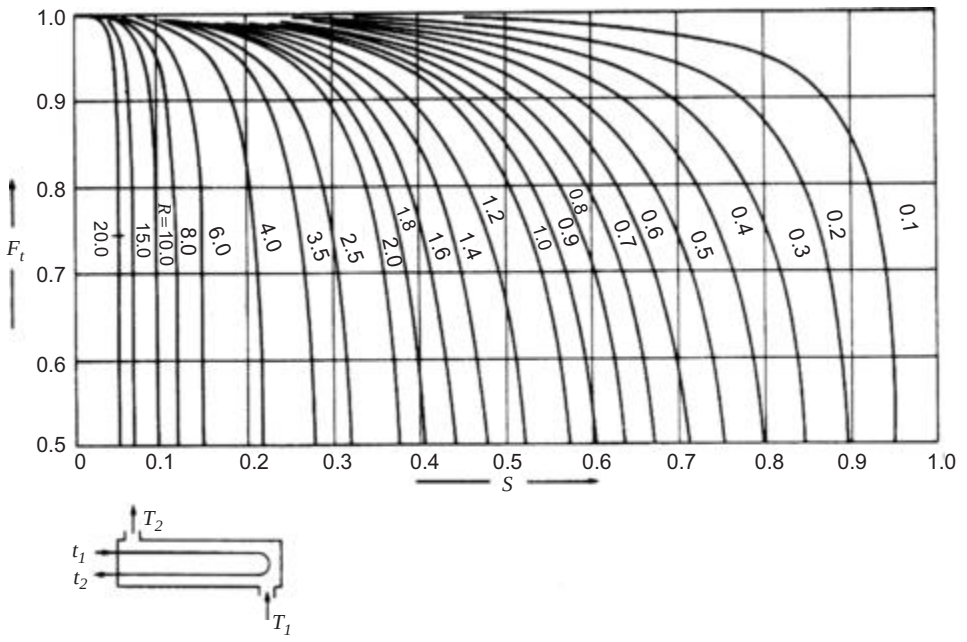


FIG. 19.19 Temperature correction factor: one-shell pass; two or more even-tube passes.

where ΔT_m = true temperature difference, the mean temperature difference for use in the design in Equation 19.1
F_t = the temperature correction factor

The correction factor is a function of the shell and tube fluid temperatures and the number of tube and shell passes. It is normally correlated as a function of two dimensionless temperature ratios:

$$R = \frac{(T_1 - T_2)}{(t_2 - t_1)} \tag{19.6}$$

and

$$S = \frac{(t_2 - t_1)}{(T_1 - t_1)} \tag{19.7}$$

R is equal to the shell-side fluid flow rate times the fluid mean specific heat divided by the tube-side fluid flow rate times the tube-side fluid specific heat.

S is a measure of the temperature efficiency of the exchanger.

For a 1 shell:2 tube pass exchanger, the correction factor is given by:

$$F_t = \frac{\sqrt{(R^2+1)}\ln\left[\dfrac{(1-S)}{(1-RS)}\right]}{(R-1)\ln\left[\dfrac{2-S\left[R+1-\sqrt{(R^2+1)}\right]}{2-S\left[R+1+\sqrt{(R^2+1)}\right]}\right]} \tag{19.8}$$

The derivation of Equation 19.8 is given by Kern (1950). The equation for a 1 shell:2 tube pass exchanger can be used for any exchanger with an even number of tube passes and is plotted in Fig. 19.19. The correction factor for two shell passes and four, or multiples of four, tube passes is shown in Fig. 19.20 and that for divided and split-flow shells in Figs. 19.21 and 19.22.

Temperature correction factor plots for other arrangements can be found in the TEMA standards and the books by Kern (1950) and Coker (2015). Mueller (1973) gives a comprehensive set of figures for calculating the log mean temperature correction factor, which includes figures for cross-flow exchangers.

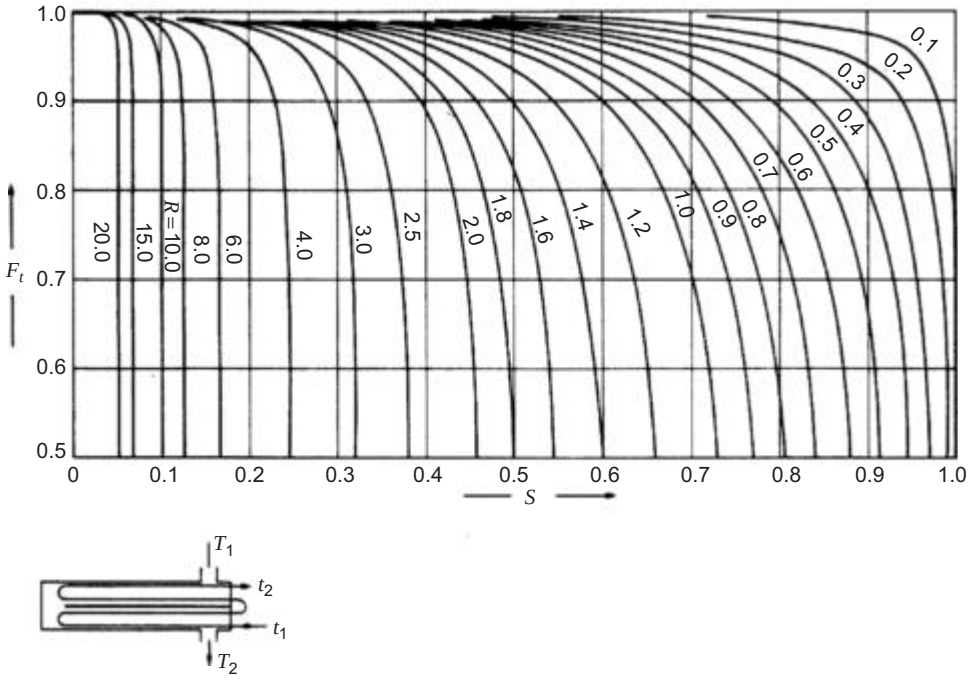


FIG. 19.20 Temperature correction factor: two-shell passes; four or multiples of four tube passes.

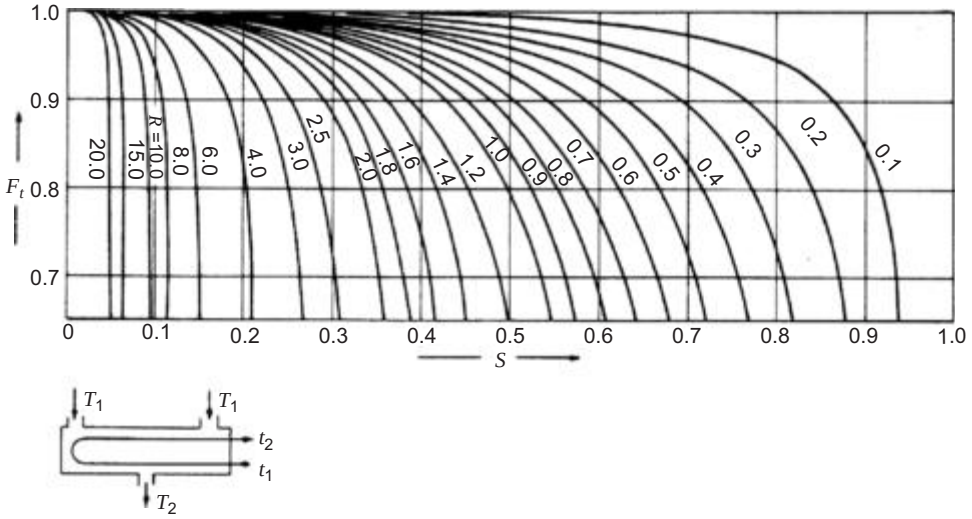


FIG. 19.21 Temperature correction factor: divided-flow shell; two or more even-tube passes.

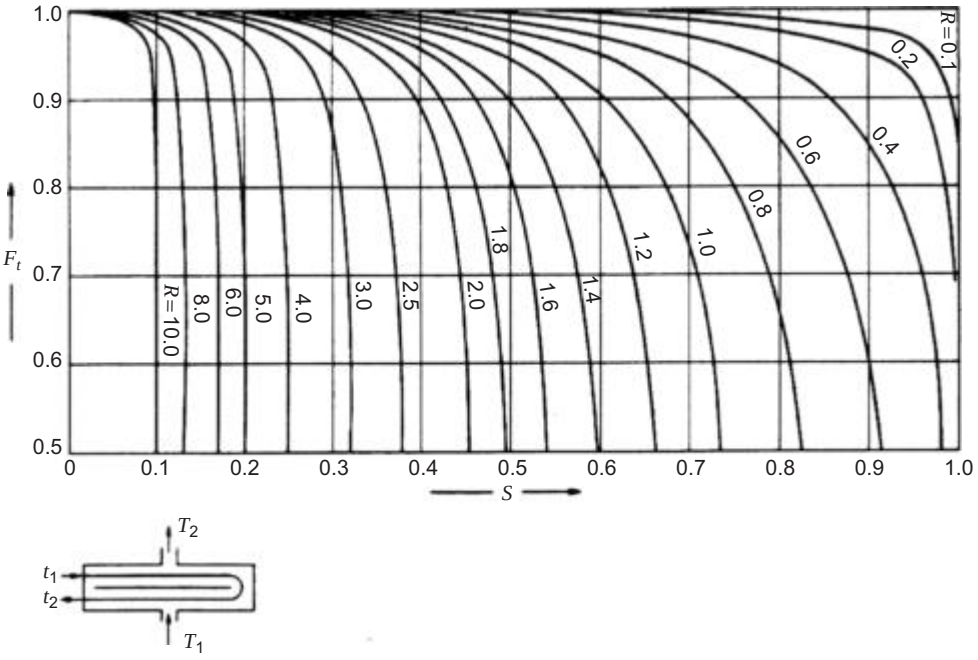


FIG. 19.22 Temperature correction factor, split-flow shell, two-tube pass.

The following assumptions are made in the derivation of the temperature correction factor, F_t, in addition to those made for the calculation of the log mean temperature difference:

1. Equal heat transfer areas in each pass.
2. A constant overall heat transfer coefficient in each pass.
3. The temperature of the shell-side fluid in any pass is constant across any cross-section.
4. There is no leakage of fluid between shell passes.

Though these conditions will not be strictly satisfied in practical heat exchangers, the F_t values obtained from the curves will give an estimate of the "true mean temperature difference" that is sufficiently accurate for most designs. Mueller (1973) discusses these assumptions and gives F_t curves for conditions when all the assumptions are not met; see also Butterworth (1973) and Emerson (1973). Values of F_t are calculated for heat exchangers in most process simulation programs, as described in Chapter 4.

The shell-side leakage and bypass streams (see Section 19.9) will affect the mean temperature difference, but are not normally taken into account when estimating the correction factor F_t. Fisher and Parker (1969) give curves that show the effect of leakage on the correction factor for a one shell pass:two tube pass exchanger.

The value of F_t will be close to 1 when the terminal temperature differences are large, but will appreciably reduce the logarithmic mean temperature difference when the temperatures of shell and tube fluids approach each other; it will fall drastically when there is a temperature cross. A temperature cross will occur if the outlet temperature of the cold stream is greater than the outlet temperature of the hot stream (see Fig. 19.18c).

Where the F_t curve is near vertical, values cannot be read accurately, which will introduce a considerable uncertainty into the design.

An economic exchanger design cannot normally be achieved if the correction factor F_t falls below about 0.75. In these circumstances, an alternative type of exchanger should be considered that gives a closer approach to true countercurrent flow. The use of two or more shells in series, or multiple shell-side passes, will give a closer approach to true countercurrent flow and should be considered where a temperature cross is likely to occur.

When both sensible and latent heat are transferred, it will be necessary to divide the temperature profile into sections and calculate the mean temperature difference for each section. The overall heat transfer coefficient should also be different in each section.

19.7 Shell and tube exchangers: General design considerations

19.7.1 Fluid allocation: Shell or tubes

Where no phase change occurs, the following factors determine the allocation of the fluid streams to the shell or tubes.

Corrosion. The more corrosive fluid should be allocated to the tube side. This will reduce the cost of expensive alloy or clad components.

Fouling. The fluid that has the greatest tendency to foul the heat transfer surfaces should be placed in the tubes. This gives better control over the design fluid velocity, and the higher allowable velocity in the tubes will reduce fouling. Also, the tubes will be easier to clean.

Fluid temperatures. If the temperatures are high enough to require the use of special alloys, placing the higher-temperature fluid in the tubes will reduce the overall cost. At moderate temperatures, placing the hotter fluid in the tubes will reduce the shell surface temperatures and hence the need for lagging to reduce heat loss, or for safety reasons.

Operating pressures. The higher-pressure stream should be allocated to the tube side. High-pressure tubes will be cheaper than a high-pressure shell. The required tube thickness is less for high internal pressure than high external pressure, and an expensive high-pressure shell may be avoided.

Pressure drop. For the same pressure drop, higher heat transfer coefficients will be obtained on the tube side than the shell side, and fluid with the lowest allowable pressure drop should be allocated to the tube side.

Viscosity. Generally, a higher heat transfer coefficient will be obtained by allocating the more viscous material to the shell side, provided the flow is turbulent. The critical Reynolds number for turbulent flow in the shell is in the region of 200. If turbulent flow cannot be achieved in the shell, it is better to place the fluid in the tubes, as the tube-side heat transfer coefficient can be predicted with more certainty.

Stream flow rates. Allocating the fluids with the lowest flow rate to the shell side will normally give the most economical design.

19.7.2 Shell and tube fluid velocities

High velocities will give high heat transfer coefficients but also a high pressure drop. The velocity must be high enough to prevent any suspended solids settling, but not so high as to cause erosion. High velocities will reduce fouling. Plastic inserts are sometimes used to reduce erosion at the tube inlet. Typical design velocities are given next.

Liquids

Tube-side process fluids: 1 to 2 m/s, maximum 4 m/s if required to reduce fouling; water: 1.5 to 2.5 m/s. Shell side: 0.3 to 1 m/s.

Vapors

For vapors, the velocity used will depend on the operating pressure and fluid density; the lower values in the ranges given here will apply to high-molecular-weight materials.

Vacuum	50 to 70 m/s
Atmospheric pressure	10 to 30 m/s
High pressure	5 to 10 m/s

19.7.3 Stream temperatures

The closer the temperature approach used (the difference between the temperatures of the two streams at a given point, usually calculated at the two ends of the exchanger), the larger the heat transfer area required for a given duty. The optimum value depends on the application and can only be determined by making an economic analysis of alternative designs. As a general guide, the optimum temperature approach will usually be in the range of 10 °C to 30 °C for heat exchange between process streams. Lower-temperature approaches are used for coolers, and a temperature approach of 5 °C to 7 °C for coolers using cooling water and 3 °C to 5 °C using refrigerated brines is common. The maximum temperature rise in recirculated cooling water is limited to around 30 °C. Care should be taken to ensure that cooling media temperatures are kept well above the freezing point of the process materials. Temperature approaches as low as 1 °C or 2 °C are used in very low-temperature subambient processes, such as air separation and natural gas liquefaction. When the heat exchange is between process fluids for heat recovery, the optimum approach temperature can be determined by pinch analysis, as described in Chapter 3. The optimum temperature approach for heat recovery depends on the trade-off between capital and energy costs (see Fig. 3.16). The numerical optimum temperature approach is seldom lower than 20 °C, but lower values are often used, as lower-temperature approaches lead to more conservative designs with more exchanger area and greater potential heat recovery.

19.7.4 Pressure drop

In many applications, the pressure drop available to drive the fluids through the exchanger will be set by the process conditions, and the available pressure drop will vary from a few millibars in vacuum service to several bars in pressure systems.

When the designer is free to select the pressure drop, an economic analysis can be made to determine the exchanger design that gives the lowest operating costs, taking into consideration both capital and pumping costs; however, a full economic analysis will only be justified for very large, expensive exchangers. The values suggested below can be used as a general guide and will normally give designs that are near the optimum.

Liquids

Viscosity	Allowable pressure drop
<1 mN s/m^2	35 kN/m^2
1–10 mN s/m^2	50–70 kN/m^2

Gas and vapors

High vacuum	0.4–0.8 kN/m^2
Medium vacuum	0.1 × absolute pressure
1–2 bar	0.5 × system gauge pressure
Above 10 bar	0.1 × system gauge pressure

When a high pressure drop is used, care must be taken to ensure that the resulting high fluid velocity does not cause erosion or flow-induced tube vibration.

19.7.5 Fluid physical properties

The fluid physical properties required for heat exchanger design are density, viscosity, thermal conductivity, and temperature–enthalpy correlations (specific and latent heats). Physical properties are usually obtained from a process simulation model; see Chapter 4. The thermal conductivities of commonly used tube materials are given in Table 19.6.

In the correlations used to predict heat transfer coefficients, the physical properties are usually evaluated at the mean stream temperature. This is satisfactory when the temperature change is small, but can cause a significant error when the change in temperature is large. In these circumstances, a simple and safe procedure is to evaluate the heat transfer coefficients at the stream inlet and outlet temperatures and use the lower of the two values. Alternatively, the method suggested by Frank (1978) can be used, in which Equations 19.1 and 19.3 are combined:

$$Q = \frac{A[U_2(T_1 - t_2) - U_1(T_2 - t_1)]}{\ln\left[\frac{U_2(T_1 - t_2)}{U_1(T_2 - t_1)}\right]} \tag{19.9}$$

where U_1 and U_2 are evaluated at the ends of the exchanger. Equation 19.9 is derived by assuming that the heat transfer coefficient varies linearly with temperature.

If the variation in the physical properties is too large for these simple methods to be used, it will be necessary to divide the temperature–enthalpy profile into sections and evaluate the heat transfer coefficients and area required for each section.

TABLE 19.6 Conductivity of metals

Metal	Temperature (°C)	k_w(W/m°C)
Aluminum	0	202
	100	206
Brass	0	97
(70 Cu, 30 Zn)	100	104
	400	116
Copper	0	388
	100	378
Nickel	0	62
	212	59
Cupro-nickel (10% Ni)	0–100	45
Monel	0–100	30
Stainless steel (18/8)	0–100	16
Carbon steel	40	60
	100	58
	260	51
Titanium	0–100	16

19.8 Tube-side heat transfer coefficient and pressure drop (single phase)

19.8.1 Heat transfer

Turbulent flow

Heat transfer data for turbulent flow inside conduits of uniform cross-section are usually correlated by an equation of the form:

$$\mathrm{Nu} = C\,\mathrm{Re}^{a}\,\mathrm{Pr}^{b}\left(\frac{\mu}{\mu_w}\right)^{c} \tag{19.10}$$

where Nu = Nusselt number = $(h_i d_e/k_f)$
Re = Reynolds number = $(\rho\, u_t d_e/\mu) = (G_t d_e/\mu)$
Pr = Prandtl number = $(C_{p\mu}/k_f)$
h_i = inside coefficient, W/m^2°C
d_e = equivalent (or hydraulic mean) diameter, m

$$d_e = \frac{4 \times \text{cross-sectional area for flow}}{\text{wetted perimeter}} = d_i \text{ for tubes,}$$

u_t = fluid velocity, m/s
k_f = fluid thermal conductivity, W/m°C
G_t = mass velocity, mass flow per unit area, kg/m^{2}s
μ = fluid viscosity at the bulk fluid temperature, Ns/m^2
μ_w = fluid viscosity at the wall
C_p = fluid-specific heat, heat capacity, J/kg°C

The index for the Reynolds number, a, is generally taken as 0.8. That for the Prandtl number, b, can range from 0.3 for cooling to 0.4 for heating. The index for the viscosity factor, c, is normally taken as 0.14 for flow in tubes, from the work of Sieder and Tate (1936), but some workers report higher values. A general equation that can be used for exchanger design is:

$$\mathrm{Nu} = C\,\mathrm{Re}^{0.8}\,\mathrm{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.11}$$

where C = 0.021 for gases
= 0.023 for nonviscous liquids
= 0.027 for viscous liquids

It is not possible to find values for the constant and indices to cover the complete range of process fluids, from gases to viscous liquids, but the values predicted using Equation 19.11 should be sufficiently accurate for design purposes. The uncertainty in the prediction of the shell-side coefficient and fouling factors will usually far outweigh any error in the tube-side value. Where a more accurate prediction than that given by Equation 19.11 is required, and justified, the data and correlations given in the Engineering Science Data Unit (ESDU) reports are recommended: ESDU 92003 and 93018 (1998).

Butterworth (1977) gives the following equation, which is based on the ESDU work:

$$\mathrm{St} = E\mathrm{Re}^{-0.205}\mathrm{Pr}^{-0.505} \tag{19.12}$$

where St = Stanton number = $(\mathrm{Nu}/\mathrm{RePr}) = (h_i/\rho u_t C_p)$
and $E = 0.0225\,\exp(-0.0225(\ln \mathrm{Pr})^2)$

Equation 19.12 is applicable at Reynolds numbers greater than 10,000.

Hydraulic mean diameter

In some texts the equivalent (hydraulic mean) diameter is defined differently for use in calculating the heat transfer coefficient in a conduit or channel than for calculating the pressure drop. The perimeter through which the heat is transferred is used in place of the total wetted perimeter. In practice, the use of d_e calculated either

way will make little difference to the value of the estimated overall coefficient, as the film coefficient is only roughly proportional to $d_e^{-0.2}$.

It is the full wetted perimeter that determines the flow regime and the velocity gradients in a channel. So, in this book, d_e determined using the full wetted perimeter will be used for both pressure drop and heat transfer calculations. The actual area through which the heat is transferred should, of course, be used to determine the rate of heat transfer (Equation 19.1).

Laminar flow

Below a Reynolds number of about 2000, the flow in pipes will be laminar. Providing the natural convection effects are small, which will normally be so in forced convection, the following equation can be used to estimate the film heat transfer coefficient:

$$\mathrm{Nu} = 1.86\,(\mathrm{RePr})^{0.33}\left(\frac{d_e}{L}\right)^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.13}$$

where L is the length of the tube in meters.

If the Nusselt number given by Equation 19.13 is less than 3.5, it should be taken as 3.5.

In laminar flow, the length of the tube can have a marked effect on the heat transfer rate for length-to-diameter ratios less than 500.

Transition region

In the flow region between laminar and fully developed turbulent flow, heat transfer coefficients cannot be predicted with certainty, as the flow in this region is unstable. The transition region should be avoided in exchanger design. If this is not practicable, the coefficient should be evaluated using both Equations 19.11 and 19.13 and the lower value taken.

Heat transfer factor, j_h

It is often convenient to correlate heat transfer data in terms of a heat transfer "j" factor, which is similar to the friction factor used for pressure drop. The heat transfer factor is defined by:

$$j_h = \mathrm{StPr}^{0.67}\left(\frac{\mu}{\mu_w}\right)^{-0.14} \tag{19.14}$$

The use of the j_h factor allows data for laminar and turbulent flow to be represented on the same graph (Fig. 19.23). The j_h values obtained from Fig. 19.23 can be used with Equation 19.14 to estimate the heat transfer coefficients for heat exchanger tubes and commercial pipes. The coefficient estimated for pipes will normally be conservative (on the low side), as pipes are rougher than the tubes used for heat exchangers, which are finished to closer tolerances. Equation 19.14 can be rearranged to a more convenient form:

$$\frac{h_i d_i}{k_f} = j_h\,\mathrm{RePr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.15}$$

Note. Kern (1950) and others define the heat transfer factor as:

$$j_H = \mathrm{NuPr}^{-1/3}\left(\frac{\mu}{\mu_w}\right)^{-0.14}$$

The relationship between j_h and j_H is given by:

$$j_H = j_h\,\mathrm{Re}$$

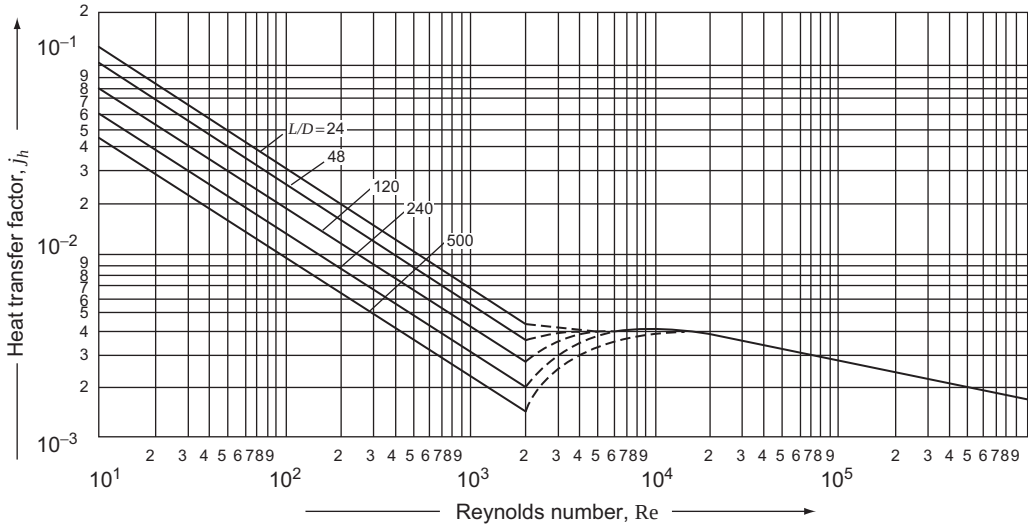


FIG. 19.23 Tube-side heat transfer factor.

Viscosity correction factor

The viscosity correction factor will normally only be significant for viscous liquids. To apply the correction, an estimate of the wall temperature is needed. This can be made by first calculating the coefficient without the correction and using the following relationship to estimate the wall temperature:

$$h_i(t_w - t) = U(T - t) \tag{19.16}$$

where t = tube-side bulk temperature (mean)
t_w = estimated wall temperature
T = shell-side bulk temperature (mean)

Usually an approximate estimate of the wall temperature is sufficient, but trial-and-error calculations can be made to obtain a better estimate if the correction is large.

Coefficients for water

Though Equations 19.11 and 19.13 and Fig. 19.23 may be used for water, a more accurate estimate can be made by using equations developed specifically for water. The physical properties are conveniently incorporated into the correlation. The following equation has been adapted from data given by Eagle and Ferguson (1930):

$$h_i = \frac{4200(1.35 + 0.02t)u_t^{0.8}}{d_i^{0.2}} \tag{19.17}$$

where h_i = inside coefficient for water, W/m^2°C
t = water temperature, °C
u_t = water velocity, m/s
d_i = tube inside diameter, mm

19.8.2 Tube-side pressure drop

There are two major sources of pressure loss on the tube side of a shell and tube exchanger: the friction loss in the tubes and the losses due to the sudden contraction and expansion and flow reversals that the fluid experiences in flow through the tube arrangement.

The tube friction loss can be calculated using the familiar equations for pressure drop in pipes (see Chapter 20). The basic equation for isothermal flow in pipes (constant temperature) is:

$$\Delta P = 8 j_f \left(\frac{L'}{d_i}\right) \frac{\rho u_t^2}{2} \tag{19.18}$$

where j_f is the dimensionless friction factor and L' is the effective pipe length.

The flow in a heat exchanger is clearly not isothermal, and this is allowed for by including an empirical correction factor to account for the change in physical properties with temperature. Normally only the change in viscosity is considered:

$$\Delta P = 8 j_f (L' / d_i) \rho \frac{u_t^2}{2} \left(\frac{\mu}{\mu_w}\right)^{-m} \tag{19.19}$$

where $m = 0.25$ for laminar flow, Re <2100
$= 0.14$ for turbulent flow, Re >2100

Values of j_f for heat exchanger tubes can be obtained from Fig. 19.24; commercial pipes are given in Chapter 20.

The pressure losses due to contraction at the tube inlets, expansion at the exits, and flow reversal in the headers can be a significant part of the total tube-side pressure drop. There is no entirely satisfactory method for estimating these losses. Kern (1950) suggests adding four velocity heads per pass. Frank (1978) considers this to be too high and recommends 2.5 velocity heads. Butterworth (1978) suggests 1.8. Lord et al. (1970) take the loss per pass as equivalent to a length of tube equal to 300 tube diameters for straight tubes and 200 for U-tubes, whereas Evans (1980) appears to add only 67 tube diameters per pass.

The loss in terms of velocity heads can be estimated by counting the number of flow contractions, expansions, and reversals and using the factors for pipe fittings to estimate the number of velocity heads lost. For two tube passes, there will be two contractions, two expansions, and one flow reversal. The head loss for each of these effects is contraction 0.5, expansion 1.0, and 180-degrre bend 1.5, so for two passes, the maximum loss will be:

$$2 \times 0.5 + 2 \times 1.0 + 1.5 = 4.5 \text{ velocity heads}$$
$$= \underline{\underline{2.25 \text{ per pass}}}$$

From this, it appears that Frank's recommended value of 2.5 velocity heads per pass is the most realistic value to use. Combining this factor with Equation 19.19 gives:

$$\Delta P_t = N_p \left[8 j_f \left(\frac{L}{d_i}\right) \left(\frac{\mu}{\mu_w}\right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2} \tag{19.20}$$

where ΔP_t = tube-side pressure drop, N/m^2 (Pa)
N_p = number of tube-side passes
u_t = tube-side velocity, m/s
L = length of one tube

Another source of pressure drop is the flow expansion and contraction at the exchanger inlet and outlet nozzles. This can be estimated by adding 1 velocity head for the inlet and 0.5 for the outlet, based on the nozzle velocities.

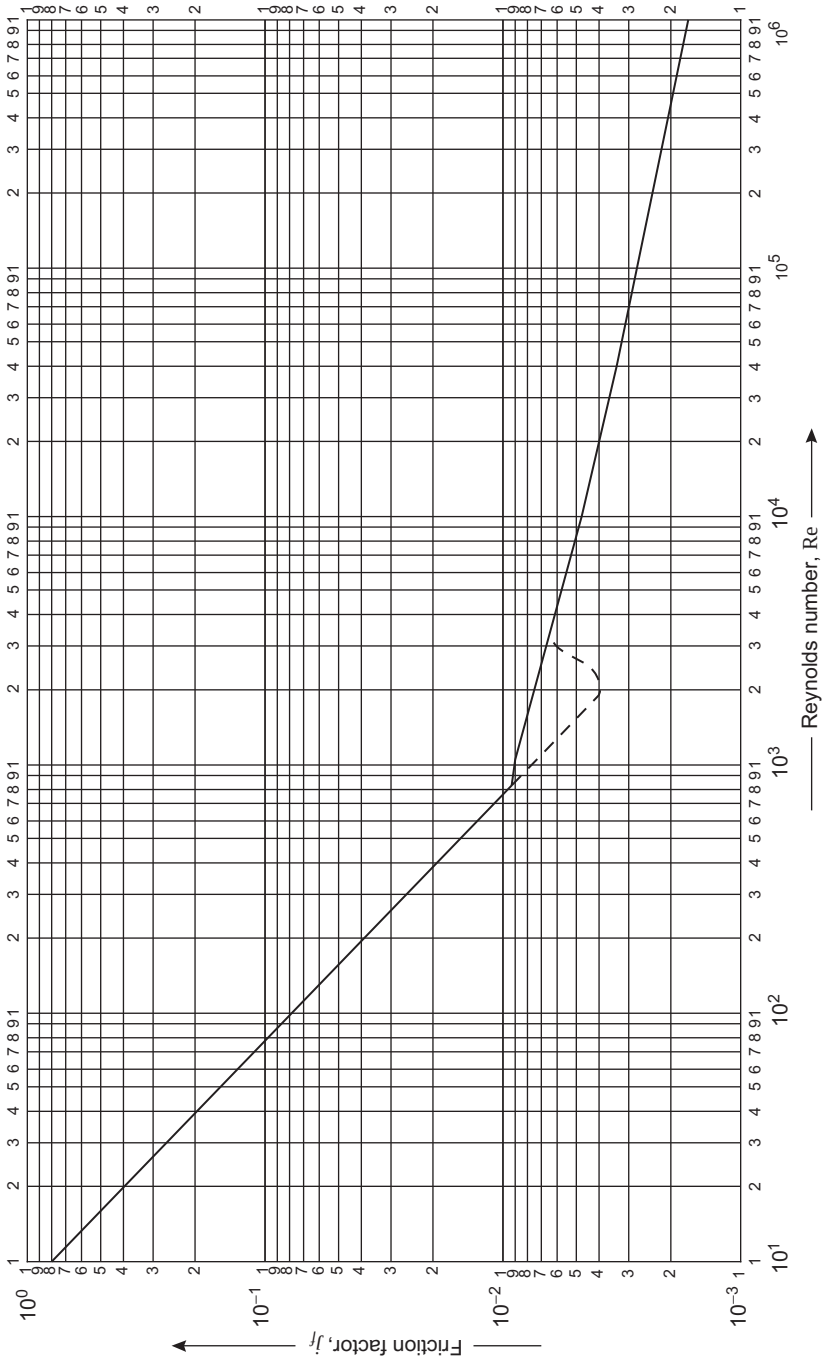


FIG. 19.24 Tube-side friction factors. *Note:* The friction factor j_f is the same as the friction factor for pipes ϕ (= $R/\rho u^2$).

19.9 Shell-side heat transfer and pressure drop (single phase)

19.9.1 Flow pattern

The flow pattern in the shell of a segmentally baffled heat exchanger is complex, and this makes the prediction of the shell-side heat transfer coefficient and pressure drop much more difficult than for the tube side. Though the baffles are installed to direct the flow across the tubes, the actual flow of the main stream of fluid will be a mixture of cross flow between the baffles, coupled with axial (parallel) flow in the baffle windows, as shown in Fig. 19.25. Not all the fluid flow follows the path shown in Fig. 19.25; some will leak through gaps formed by the clearances that have to be allowed for fabrication and assembly of the exchanger. These leakage and bypass streams are shown

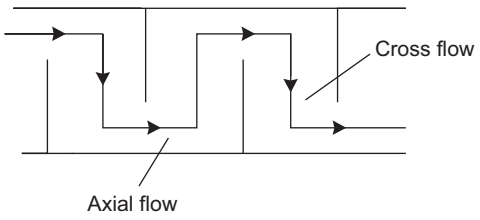


FIG. 19.25 Idealized main stream flow.

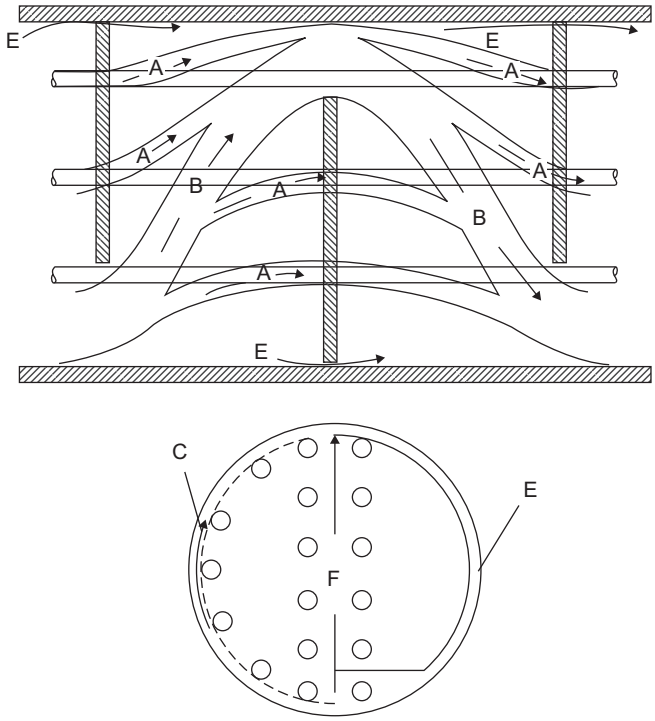


FIG. 19.26 Shell-side leakage and bypass paths.

in Fig. 19.26, which is based on the flow model proposed by Tinker (1951, 1958). In Fig. 19.26, Tinker's nomenclature is used to identify the various streams, as follows:

Stream A is the tube-to-baffle leakage stream, which is the fluid flowing through the clearance between the tube outside diameter and the tube hole in the baffle.
Stream B is the actual cross-flow stream.
Stream C is the bundle-to-shell bypass stream, which is the fluid flowing in the clearance area between the outer tubes in the bundle (bundle diameter) and the shell.
Stream E is the baffle-to-shell leakage stream, which is the fluid flowing through the clearance between the edge of a baffle and the shell wall.
Stream F is the pass-partition stream, which is the fluid flowing through the gap in the tube arrangement due to the pass partition plates. Where the gap is vertical, it will provide a low-pressure drop path for fluid flow.

Note. There is no stream D.

The fluid in streams C, E, and F bypasses the tubes, reducing the effective heat transfer area.

Stream C is the main bypass stream and is particularly significant in pull-through bundle exchangers, where the clearance between the shell and bundle is necessarily large. Stream C can be considerably reduced by using sealing strips; horizontal strips that block the gap between the bundle and the shell (Fig. 19.27). Dummy tubes are also sometimes used to block the pass-partition leakage, stream F.

The tube-to-baffle leakage stream, A, does not bypass the tubes, and its main effect is on pressure drop rather than heat transfer.

The clearances will tend to plug as the exchanger becomes fouled, and this will increase the pressure drop; see Section 19.9.6.

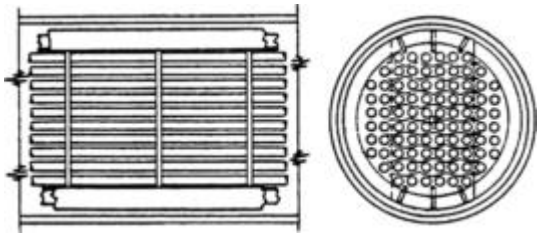


FIG. 19.27 Sealing strips.

19.9.2 Design methods

The complex flow pattern on the shell side, and the great number of variables involved, make it difficult to predict the shell-side heat transfer coefficient and pressure drop with complete assurance. In methods used for the design of exchangers before about 1960, no attempt was made to account for the leakage and bypass streams. Correlations were based on the total stream flow, and empirical methods were used to account for the performance of real exchangers compared with that for cross flow over ideal tube banks. Typical of these "bulk-flow" methods are those of Kern (1950) and Donohue (1955). Reliable predictions can only be achieved by comprehensive analysis of the contribution to heat transfer and pressure drop made by the individual streams shown in Fig. 19.26. Tinker (1951, 1958) published the first detailed stream-analysis method for predicting shell-side heat transfer coefficients and pressure drop, and the methods subsequently developed have been based on his model. Tinker's presentation is difficult to follow, and his method is difficult and tedious to apply in manual calculations. It has been simplified by Devore (1961, 1962) using standard tolerances for commercial exchangers and only a limited number of baffle cuts. Devore gives nomographs that facilitate the application of the method in manual calculations. Mueller (1973) has further simplified Devore's method and gives an illustrative example.

Bell (1960, 1963) developed a semi-analytical method based on work done in the cooperative research program on shell and tube exchangers at the University of Delaware. His method accounts for the major bypass and leakage streams and is suitable for a manual calculation.

The ESDU has also published a method for estimating shell-side the pressure drop and heat transfer coefficient: ESDU Design Guide 83038 (1984). The method is based on a simplification of Tinker's work. It can be used for hand calculations, but as iterative procedures are involved, it is best programmed for use with personal computers.

Tinker's model has been used as the basis for the proprietary computer methods developed by Heat Transfer Research Incorporated; see Palen and Taborek (1969), and by Heat Transfer and Fluid Flow Services; see Grant (1973). The HTRI method and software are available from HTRI (www.htri.net). The HTFS programs are available in process simulation programs such as Aspen Technology's Aspen Engineering Suite and Honeywell's UniSim Design Suite; see Chapter 4. The use of the HTFS programs is illustrated in Example 19.4.

Though Kern's method does not take account of the bypass and leakage streams, it is simple to apply and is accurate enough for preliminary design calculations and for designs where uncertainty in other design parameters is such that the use of more elaborate methods is not justified. Kern's method is given in Section 19.9.3 and is illustrated in Examples 19.1 and 19.3.

19.9.3 Kern's method

This method was based on experimental work on commercial exchangers with standard tolerances and will give a reasonably satisfactory prediction of the heat transfer coefficient for standard designs. The prediction of pressure drop is less satisfactory, as pressure drop is more affected by leakage and bypassing than by heat transfer. The shell-side heat transfer and friction factors are correlated in a similar manner to those for tube-side flow by using a hypothetical shell velocity and shell diameter. As the cross-sectional area for flow varies across the shell diameter, the linear and mass velocities are based on the maximum area for cross flow: that at the shell equator. The shell equivalent diameter is calculated using the flow area between the tubes taken in the axial direction (parallel to the tubes) and the wetted perimeter of the tubes (Fig. 19.28).

Shell-side j_h and j_f factors for use in this method are given in Figs. 19.29 and 19.30 for various baffle cuts and tube arrangements. These figures are based on data given by Kern (1950) and by Coker (2015).

The procedure for calculating the shell-side heat transfer coefficient and pressure drop for a single shell pass exchanger is given next.

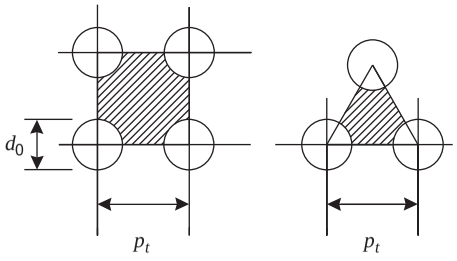


FIG. 19.28 Equivalent diameter, cross-sectional areas, and wetted perimeters.

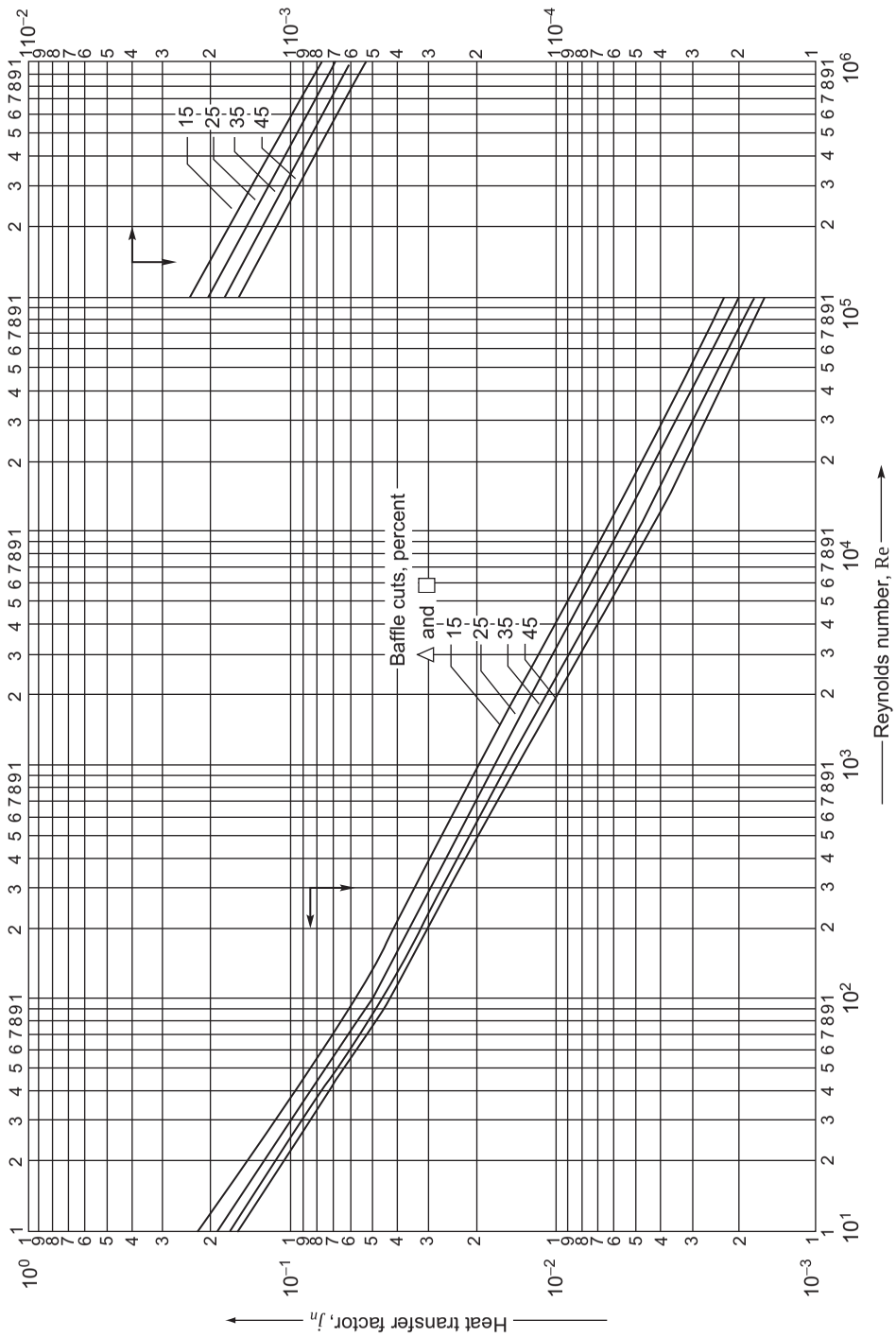


FIG. 19.29 Shell-side heat transfer factors, segmental baffles.

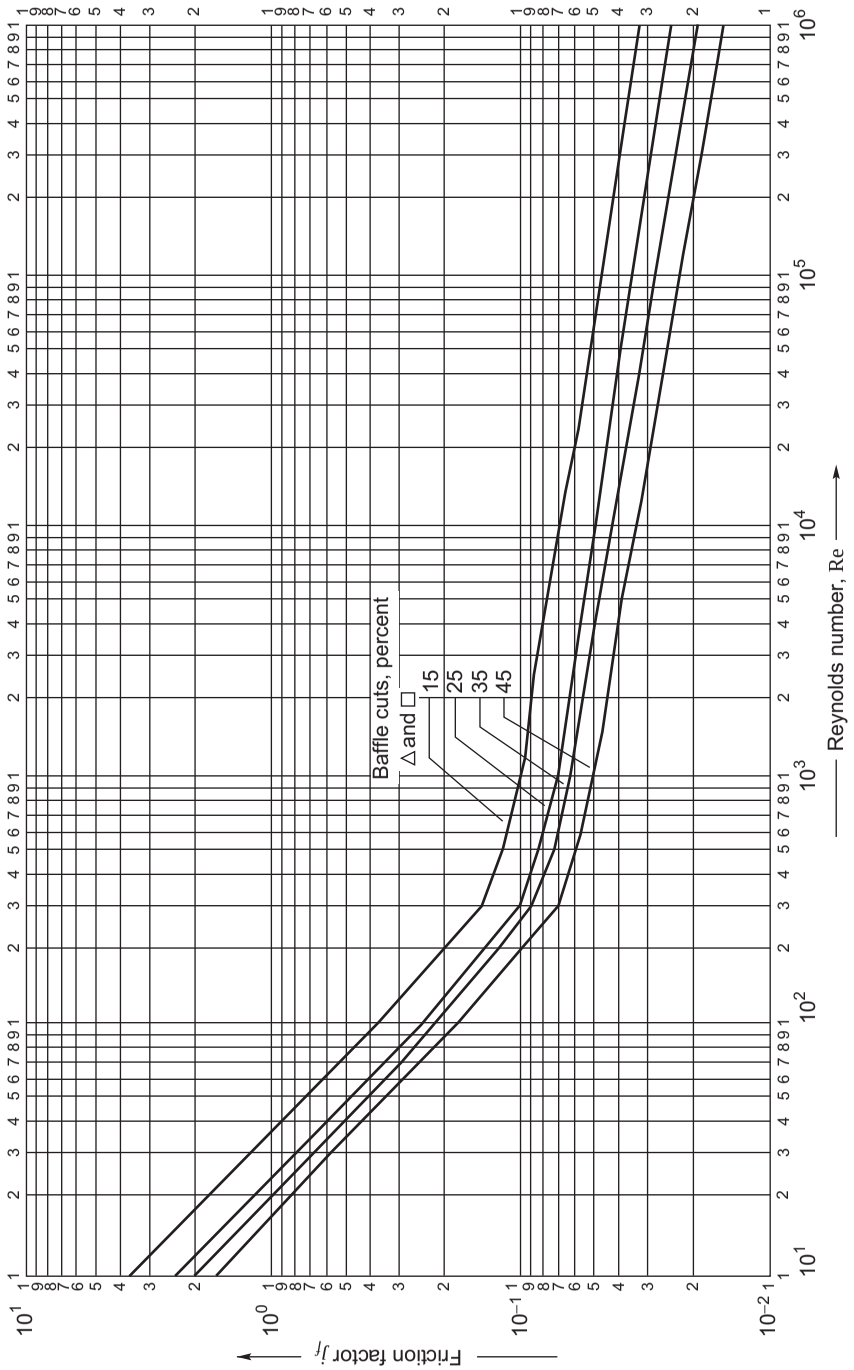


FIG. 19.30 Shell-side friction factors, segmental baffles.

Procedure

1. Calculate the area for cross-flow A_s for the hypothetical row of tubes at the shell equator, given by:

$$A_s = \frac{(p_t - d_o)D_s l_B}{p_t} \tag{19.21}$$

where p_t = tube pitch
d_o = tube outside diameter
D_s = shell inside diameter, m
l_B = baffle spacing, m

The term $(p_t - d_o)/p_t$ is the ratio of the clearance between tubes and the total distance between tube centers.

2. Calculate the shell-side mass velocity G_s and the linear velocity u_s:

$$G_s = \frac{W_s}{A_s}$$

$$u_s = \frac{G_s}{\rho}$$

where W_s = fluid flow rate on the shell side, kg/s
ρ = shell-side fluid density, kg/m^3

3. Calculate the shell-side equivalent diameter (hydraulic diameter) (see Fig. 19.28). For a square pitch arrangement:
For an equilateral triangular pitch arrangement:

$$d_e = \frac{4\left(\frac{p_t^2 - \pi d_o^2}{4}\right)}{\pi d_o} = \frac{1.27}{d_o}\left(p_t^2 - 0.785 d_o^2\right) \tag{19.22}$$

$$d_e = \frac{4\left(\frac{p_t}{2} \times 0.87\, p_t - \frac{1}{2}\pi\frac{d_o^2}{4}\right)}{\frac{\pi d_o}{2}} = \frac{1.10}{d_o}\left(p_t^2 - 0.917 d_o^2\right) \tag{19.23}$$

where d_e = equivalent diameter, m.

4. Calculate the shell-side Reynolds number, given by:

$$\mathrm{Re} = \frac{G_s d_e}{\mu} = \frac{u_s d_e \rho}{\mu} \tag{19.24}$$

5. For the calculated Reynolds number, read the value of j_h from Fig. 19.29 for the selected baffle cut and tube arrangement and calculate the shell-side heat transfer coefficient h_s from:

$$\mathrm{Nu} = \frac{h_s d_e}{k_f} = j_h\, \mathrm{RePr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.25}$$

The tube wall temperature can be estimated using the method given for the tube side; see Section 19.8.1.

6. For the calculated shell-side Reynolds number, read the friction factor from Fig. 19.30 and calculate the shell-side pressure drop from:

$$\Delta P_s = 8\, j_f \left(\frac{D_s}{d_e}\right)\left(\frac{L}{l_B}\right)\frac{\rho u_s^2}{2}\left(\frac{\mu}{\mu_w}\right)^{-0.14} \tag{19.26}$$

where L = tube length
l_B = baffle spacing

The term (L/l_B) is the number of times the flow crosses the tube bundle = $(N_b + 1)$, where N_b is the number of baffles.

Shell nozzle-pressure drop

The pressure loss in the shell nozzles will normally only be significant with gases. The nozzle pressure drop can be taken as equivalent to 1½ velocity heads for the inlet and ½ for the outlet, based on the nozzle area or the free area between the tubes in the row immediately adjacent to the nozzle, whichever is the lower.

Example 19.1

Design an exchanger to subcool condensate from a methanol condenser from 95 °C to 40 °C. The flow rate of methanol is 100,000 kg/h. Brackish water will be used as the coolant, with a temperature rise from 25 °C to 40 °C.

Solution

Only the thermal design will be considered. This example illustrates Kern's method. Coolant is corrosive, so assign to tube side:

$$\text{Heat capacity methanol} = 2.84 \text{ kJ/kg}^{\circ}\text{C}$$

$$\text{Heat load} = \frac{100,000}{3600} \times 2.84(95-40) = 4340 \text{ kW}$$

$$\text{Heat capacity water} = 4.2 \text{ kJ/kg}^{\circ}\text{C}$$

$$\text{Cooling water flow} = \frac{4340}{4.2(40-25)} = 68.9 \text{ kg/s}$$

$$\Delta T_{\text{lm}} = \frac{(95-40)-(40-25)}{\ln\dfrac{(95-40)}{(40-25)}} = 31^{\circ}\text{C} \tag{19.4}$$

Use one shell pass and two tube passes:

$$R = \frac{95-40}{40-25} = 3.67 \tag{19.6}$$

$$S = \frac{40-25}{95-25} = 0.21 \tag{19.7}$$

From Fig. 19.19:

$$F_t = 0.85$$

$$\Delta T_m = 0.85 \times 31 = 26^{\circ}\text{C}$$

From Fig. 19.1:

$$\text{U} = 600 \text{ W/m}^{2^{\circ}}\text{C}$$

Provisional area:

$$A = \frac{4340 \times 10^3}{26 \times 600} = 278 \text{ m}^2 \tag{19.1}$$

Choose 20 mm o.d., 16 mm i.d., 4.88-m-long tubes (¾ in. × 16 ft), cupro-nickel.
Allowing for tubesheet thickness, take:

$$\text{L} = 4.83 \text{ m}$$

$$\text{Area of one tube} = 4.83 \times 20 \times 10^{-3}\pi = 0.303 \text{ m}^2$$

$$\text{Number of tubes} = \frac{278}{0.303} = \underline{\underline{918}}$$

As the shell-side fluid is relatively clean, use 1.25 triangular pitch:

$$\text{Bundle diameter } D_b = 20\left(\frac{918}{0.249}\right)^{1/2.207} = 826 \text{ mm} \tag{19.3b}$$

Use a split-ring floating head type.
From Fig. 19.10, bundle diametrical clearance = 68 mm and shell diameter, $D_s = 826 + 68 = 894$ mm. (*Note:* The nearest standard pipe sizes are 863.6 or 914.4 mm.) The shell size could be read from standard tube count tables.

Tube-side coefficient

$$\text{Mean water temperature} = \frac{40+25}{2} = 33^{\circ}\text{C}$$

$$\text{Tube cross} - \text{sectional area} = \frac{\pi}{4} \times 16^2 = 201 \text{ mm}^2$$

$$\text{Tubes per pass} = \frac{918}{2} = 459$$

$$\text{Total flow area} = 459 \times 201 \times 10^{-6} = 0.092 \text{ m}^2$$

$$\text{Water mass velocity} = \frac{68.9}{0.092} = 749 \text{ kg/s m}^2$$

$$\text{Density water} = 995 \text{ kg/m}^3$$

$$\text{Water linear velocity} = \frac{749}{995} = 0.75 \text{ m/s}$$

$$h_i = \frac{4200(1.35 + 0.02 \times 33)0.75^{0.8}}{16^{0.2}} = 3852 \text{ W/m}^{2^{\circ}}\text{C} \tag{19.17}$$

The coefficient can also be calculated using Equation 19.15; this is done to illustrate use of this method.

$$\frac{h_i d_i}{k_f} = j_h Re Pr^{0.33} \left(\frac{\mu}{\mu_w}\right)^{0.14}$$

$$\text{Viscosity of water} = 0.8 \text{ mNs/m}^2$$

$$\text{Thermal conductivity} = 0.59 \text{W/m}^{\circ}\text{C}$$

$$\text{Re} = \frac{\rho u d_i}{\mu} = \frac{995 \times 0.75 \times 16 \times 10^{-3}}{0.8 \times 10^{-3}} = 14,925$$

$$\text{Pr} = \frac{C_p \mu}{k_f} = \frac{4.2 \times 10^3 \times 0.8 \times 10^{-3}}{0.59} = 5.7$$

$$\text{Neglect } \left(\frac{\mu}{\mu_w}\right)$$

$$\frac{L}{d_i} = \frac{4.83 \times 10^3}{16} = 302$$

From Fig. 19.23, $j_h = 3.9 \times 10^{-3}$.

$$h_i = \frac{0.59}{16 \times 10^{-3}} \times 3.9 \times 10^{-3} \times 14,925 \times 5.7^{0.33} = 3812 \text{ W/m}^{2^{\circ}}\text{C}$$

Checks reasonably well with value calculated from Equation 19.17; use lower figure.

Shell-side coefficient

$$\text{Choose baffle spacing} = \frac{D_s}{5} = \frac{894}{5} = 178 \text{ mm.}$$

$$\text{Tube pitch} = 1.25 \times 20 = 25 \text{ mm}$$

$$\text{Cross-flow area } A_s = \frac{(25-20)}{25} 894 \times 178 \times 10^{-6} = 0.032 \text{ m}^2 \tag{19.21}$$

$$\text{Mass velocity, } G_s = \frac{100,000}{3600} \times \frac{1}{0.032} = 868 \text{ kg/s m}^2$$

$$\text{Equivalent diameter } d_e = \frac{1.1}{20}\left(25^2 - 0.917 \times 20^2\right) = 14.4 \text{ mm} \tag{19.23}$$

$$\text{Mean shell side temperature} = \frac{95+40}{2} = 68^\circ\text{C}$$

$$\text{Methanol density} = 750 \text{ kg/m}^3$$

$$\text{Viscosity} = 0.34 \text{ mNs/m}^2$$

$$\text{Heat capacity} = 2.84 \text{ kJ/kg}^\circ\text{C}$$

$$\text{Thermal conductivity} = 0.19 \text{ W/m}^\circ\text{C}$$

$$\text{Re} = \frac{G_s d_e}{\mu} = \frac{868 \times 14.4 \times 10^{-3}}{0.34 \times 10^{-3}} = 36,762 \tag{19.24}$$

$$\text{Pr} = \frac{C_p \mu}{k_f} = \frac{2.84 \times 10^3 \times 0.34 \times 10^{-3}}{0.19} = 5.1$$

Choose a 25% baffle cut from Fig. 19.29:

$$j_h = 3.3 \times 10^{-3}$$

Without viscosity correction term:

$$h_s = \frac{0.19}{14.4 \times 10^{-3}} \times 3.3 \times 10^{-3} \times 36,762 \times 5.1^{1/3} = 2740 \text{ W/m}^{2\circ}\text{C}$$

Estimate wall temperature:

$$\text{Mean temperature difference} = 68 - 33 = 35^\circ\text{C}$$

$$\text{across all resistances}$$

$$\text{across methanol film} = \frac{U}{h_o} \times \Delta T = \frac{600}{2740} \times 35 = 8^\circ\text{C}$$

Mean wall temperature $= 68 - 8 = 60$ °C:

$$\mu_w = 0.37 \text{ mNs/m}^2$$

$$\left(\frac{\mu}{\mu_w}\right)^{0.14} = 0.99$$

which shows that the correction for a low-viscosity fluid is not significant.

Overall coefficient

Thermal conductivity of cupro-nickel alloys = 50 W/m°C.

Take the fouling coefficients from Table 19.2: methanol (light organic) 5000 W/m$^{2^\circ}$C, brackish water (sea water), take as highest value 3000 W/m$^{2^\circ}$C:

$$\frac{1}{U_o} = \frac{1}{2740} + \frac{1}{5000} + \frac{20 \times 10^{-3} \ln\left(\frac{20}{16}\right)}{2 \times 50} + \frac{20}{16} \times \frac{1}{3000} + \frac{20}{16} \times \frac{1}{3812} \tag{19.2}$$

$$U_o = \underline{\underline{738 \text{ W/m}^{2^\circ}\text{C}}}$$

Well above the assumed value of 600 W/m$^{2^\circ}$C.

Pressure drop: Tube-side

From Fig. 19.24, for Re = 14,925:

$$j_f = 4.3 \times 10^{-3}$$

Neglecting the viscosity correction term:

$$\Delta P_t = 2\left(8\times 4.3\times 10^{-3}\left(\frac{4.83\times 10^3}{16}\right)+2.5\right)\ \frac{995\times 0.75^2}{2}$$
$$= 7211\ \text{N/m}^2 = 7.2\ \text{kPa}\ (1.1\ \text{psi}) \tag{19.20}$$

low, could consider increasing the number of tube passes.

Pressure drop: Shell side

$$\text{Linear velocity} = \frac{G_s}{\rho} = \frac{868}{750} = 1.16\ \text{m/s}$$

From Fig. 19.30, at Re = 36,762:

$$j_f = 4\times 10^{-2}$$

Neglect the viscosity correction:

$$\Delta P_s = 8\times 4\times 10^{-2}\left(\frac{894}{14.4}\right)\ \left(\frac{4.83\times 10^3}{178}\right)\ \frac{750\times 1.16^2}{2}$$
$$= 272,019\ \text{N/m}^2 \tag{19.26}$$
$$= 272\ \text{kPa}\ (39\ \text{psi})\ \text{too high,}$$

could be reduced by increasing the baffle pitch. Doubling the pitch halves the shell-side velocity, which reduces the pressure drop by a factor of approximately (½)^2:

$$\Delta P_s = \frac{272}{4} = 68\ \text{kPa}\ (10\ \text{psi}),\ \text{acceptable}$$

This will reduce the shell-side heat transfer coefficient by a factor of $(1/2)^{0.8}$ ($h_o \propto Re^{0.8} \propto u_s^{0.8}$):

$$h_o = 2740\times\left(\frac{1}{2}\right)^{0.8} = 1573\ \text{W/m}^{2\circ}\text{C}$$

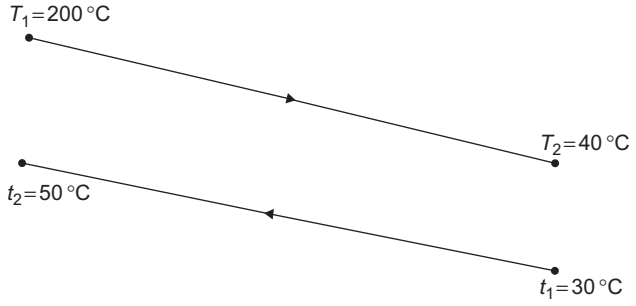
This gives an overall coefficient of 615 W/m$^{2\circ}$C, which is still above assumed value of 600 W/m$^{2\circ}$C.

Example 19.2

Gas oil at 200 °C is to be cooled to 40 °C. The oil flow rate is 22,500 kg/h. Cooling water is available at 30 °C, and the temperature rise is to be limited to 20 °C. The pressure drop allowance for each stream is 100 kN/m^2. Design a suitable exchanger for this duty.

Solution

Only the thermal design will be carried out to illustrate the calculation procedure for an exchanger with a divided shell.



$$\Delta T_{l\,m} = \frac{(200-40)-(40-30)}{\mathrm{Ln}\dfrac{(200-50)}{(40-30)}} = 51.7^{\circ}\mathrm{C} \tag{19.4}$$

$$R = (200-50)/(50-30) = 8.0 \tag{19.6}$$

$$S = (50-30)/(200-30) = 0.12 \tag{19.7}$$

These values do not intercept on the figure for a single shell-pass exchanger (see Fig. 19.19) so use the figure for a two-pass shell (see Fig. 19.20), which gives:

$$F_t = 0.94, \text{so}$$

$$\Delta T_m = 0.94 \times 51.7 = 48.6^{\circ}\mathrm{C}$$

Physical properties

Water, from steam tables:

Temperature, °C	**30**	**40**	**50**
C_p, kJ/kg°C	4.18	4.18	4.18
k, kW/m°C	618×10^{-6}	631×10^{-6}	643×10^{-6}
μ, mNm^{-2}s	797×10^{-3}	671×10^{-3}	544×10^{-3}
ρ, kg m^{-3}	995.2	992.8	990.1

Gas oil, from Kern (1950):

Temperature, °C	**200**	**120**	**40**
C_p, kJ/kg°C	2.59	2.28	1.97
k, W/m°C	0.13	0.125	0.12
μ, mNm^{-2}s	0.06	0.17	0.28
ρ, kg/m^3	830	850	870

Duty:

$$\text{Oil flow rate} = 22,500/3600 = 6.25 \text{ kg/s}$$

$$Q = 6.25 \times 2.28 \times (200 - 40) = 2280 \text{ kW}$$

$$\text{Water flow rate} = \frac{2280}{4.18(50-30)} = 27.27 \text{ kg/h}$$

From Fig. 19.1, for cooling tower water and heavy organic liquid, take:

$$U = 500 \text{ Wm}^{-2}\text{C}^{-1}$$

$$\text{Area required} = \frac{2280 \times 10^3}{500 \times 48.6} = 94 \text{ m}^2$$

Tube-side coefficient

Select 20 mm o.d., 16 mm i.d. tubes, 4 m long, triangular pitch $1.25d_o$, carbon steel.

Surface area of one tube $= \pi \times 20 \times 10^{-3} \times 4 = 0.251$ m^2

Number of tubes required $= 94/0.251 = 375$; say 376, even number

Cross-sectional area, one tube $= \frac{\pi}{4}(16 \times 10^{-3})^2 = 2.011 \times 10^{-4}$ m^2

Total tube area $= 376 \times 2.011 \times 10^{-4} = 0.0756$ m^2

Put water through the tube for ease of cleaning.

Tube velocity, one pass $= 27.27/(992.8 \times 0.0756) = 0.363$ m/s

Too low to make effective use of the allowable pressure drop; try four passes.

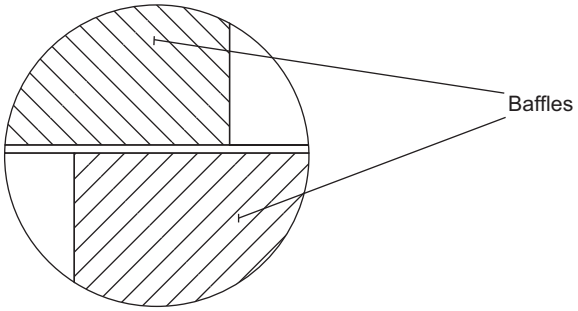
$$u_t = 4 \times 0.363 = 1.45 \text{ m/s}$$

A floating head will be needed due to the temperature difference. Use a pull-through type.
Tube-side heat transfer coefficient:

$$h_i = \frac{4200(1.35 + 0.02 \times 40)1.45^{0.8}}{16^{0.2}} = 6982 \ \text{Wm}^{-2\circ}\text{C}^{-1} \tag{19.17}$$

Shell-side coefficient

From Table 19.4 and Equation 19.3*b*, for four passes, $1.25d_o$ triangular pitch:
Bundle diameter, $D_b = 20(376/0.175)^{1/2.285} = 575$ mm
From Fig. 19.10, for pull-through head, clearance = 92 mm:
Shell diameter, $D_s = 575 + 92 = 667$ mm (26 in. pipe)
Use 25% cut baffles, with the baffle arrangement for a divided shell as shown here:



Take the baffle spacing as $\frac{1}{5}$ shell diameter $= 667/5 = 133$ mm
Tube pitch, $p_t = 1.25 \times 20 = 25$ mm
Area for flow, A_s, will be half that given by Equation 19.21:

$$\begin{aligned} A_s &= 0.5 \times \left(\frac{25-20}{25} \times 0.667 \times 0.133\right) = 0.00887 \ \text{m}^2 \\ G_s &= 6.25/0.00887 = 704.6 \ \text{kg/s} \\ u_s &= 704.6/850 = 0.83 \ \text{m/s}, \ \text{looks reasonable} \\ d_e &= \frac{1.10}{20}\left(25^2 - 0.917 \times 20^2\right) = 14.2 \ \text{mm} \\ \text{Re} &= \frac{0.83 \times 14.2 \times 10^{-3} \times 850}{0.17 \times 10^{-3}} = 58,930 \end{aligned} \tag{19.23}$$

From Fig. 19.29, $j_h = 2.6 \times 10^{-3}$:

$$\begin{aligned} \text{Pr} &= \left(2.28 \times 10^3 \times 0.17 \times 10^{-3}\right)/0.125 = 3.1 \\ \text{Nu} &= 2.6 \times 10^{-3} \times 58,930 \times 3.1^{1/3} = 223.4 \\ h_s &= (223.4 \times 0.125)/\left(14.2 \times 10^{-3}\right) = 1967 \ \text{W/m}^{2\circ}\text{C} \end{aligned} \tag{19.25}$$

Overall coefficient

Take fouling factors as 0.00025 for cooling tower water and 0.0002 for gas oil (light organic). Thermal conductivity for carbon steel tubes 45 W/m°C:

$$\begin{aligned} 1/U_o &= 1/1967 + 0.0002 + \frac{20 \times 10^{-3} \ln(20/16)}{2 \times 45} + 20/16(1/6982 + 0.00025) = 0.00125 \\ U_o &= 1/0.00125 = 800 \ \text{Wm}^{-2\circ}\text{C}^{-1} \end{aligned} \tag{19.2}$$

Well above the initial estimate of 500 W/m$^{2\circ}$C, so design has adequate area for the duty required.

Pressure drops: Tube side

$$\mathrm{Re} = \frac{1.45 \times 16 \times 10^{-3} \times 992.8}{670 \times 10^{-6}} = 34,378 \quad (3.4 \times 10^{-4})$$

From Fig. 19.24, $j_f = 3.5 \times 10^{-3}$. Neglecting the viscosity correction:

$$\Delta P_t = 4\left[8 \times 3.5 \times 10^{-3} \times \left(\frac{4}{16 \times 10^{-3}}\right) + 2.5\right] 992.8 \times \frac{1.45^2}{2} = 39,660$$
$$= 40\ \mathrm{kN/m^2} \tag{19.20}$$

Well within the specification, so no need to check the nozzle pressure drop.

Pressure drops: Shell side

From Fig. 19.30, for Re = 58,930, $j_f = 3.8 \times 10^{-2}$

With a divided shell, the path length $= 2 \times (L/l_b)$

Neglecting the viscosity correction factor:

$$\Delta P_s = 8 \times 3.8 \times 10^{-2} \left(\frac{662 \times 10^{-3}}{14.2 \times 10^{-3}}\right) \times \left(\frac{2 \times 4}{132 \times 10^{-3}}\right) \times 850 \times \frac{0.83^2}{2} = 251,481$$
$$= 252\ \mathrm{kN/m^2} \tag{19.26}$$

Well within the specification, no need to check nozzle pressure drops.

So the proposed thermal design is satisfactory. As the calculated pressure drops are below that allowed, there is some scope for improving the design.

Example 19.3

Design a shell and tube exchanger for the following duty.

20,000 kg/h of kerosene (42° API) leaves the base of a kerosene side-stripping column at 200 °C and is to be cooled to 90 °C by exchange with 70,000 kg/h light crude oil (34° API) coming from storage at 40 °C. The kerosene enters the exchanger at a pressure of 5 bar and the crude oil at 6.5 bar. A pressure drop of 0.8 bar is permissible on both streams. Allowance should be made for fouling by including a fouling factor of 0.0003 $(\mathrm{W/m^2\ °C})^{-1}$ on the crude stream and 0.0002 $(\mathrm{W/m^2°C})^{-1}$ on the kerosene stream.

Solution

The solution to this example illustrates the iterative nature of heat exchanger design calculations. An algorithm for the design of shell and tube exchangers is shown in Fig. 19.31. The procedure set out in this figure will be followed in the solution.

Step 1: Specification

The specification is given in the problem statement:

20,000 kg/h of kerosene (42° API) at 200 °C cooled to 90 °C by exchange with 70,000 kg/h light crude oil (34° API) at 40 °C.

The kerosene pressure is 5 bar, and the crude oil pressure is 6.5 bar.

Permissible pressure drop of 0.8 bar on both streams.

Fouling factors: crude stream 0.00035 $(\mathrm{W/m^2°C})^{-1}$, kerosene stream 0.0002 $(\mathrm{W/m^2°C})^{-1}$.

To complete the specification, the duty (heat transfer rate) and the outlet temperature of the crude oil needed to be calculated.

Mean temperature of kerosene $= (200 + 90)/2 = 145$ °C.

At this temperature, the specific heat capacity of 42° API kerosene is 2.47 kJ/kg°C (physical properties from Kern 1950).

$$\mathrm{Duty} = \frac{20,000}{3600} \times 2.47(200 - 90) = 1509.4\ \mathrm{kW}$$

As a first trial, take the mean temperature of the crude oil as equal to the inlet temperature, 40 °C; specific heat capacity at this temperature = 2.01 kJ/kg°C.

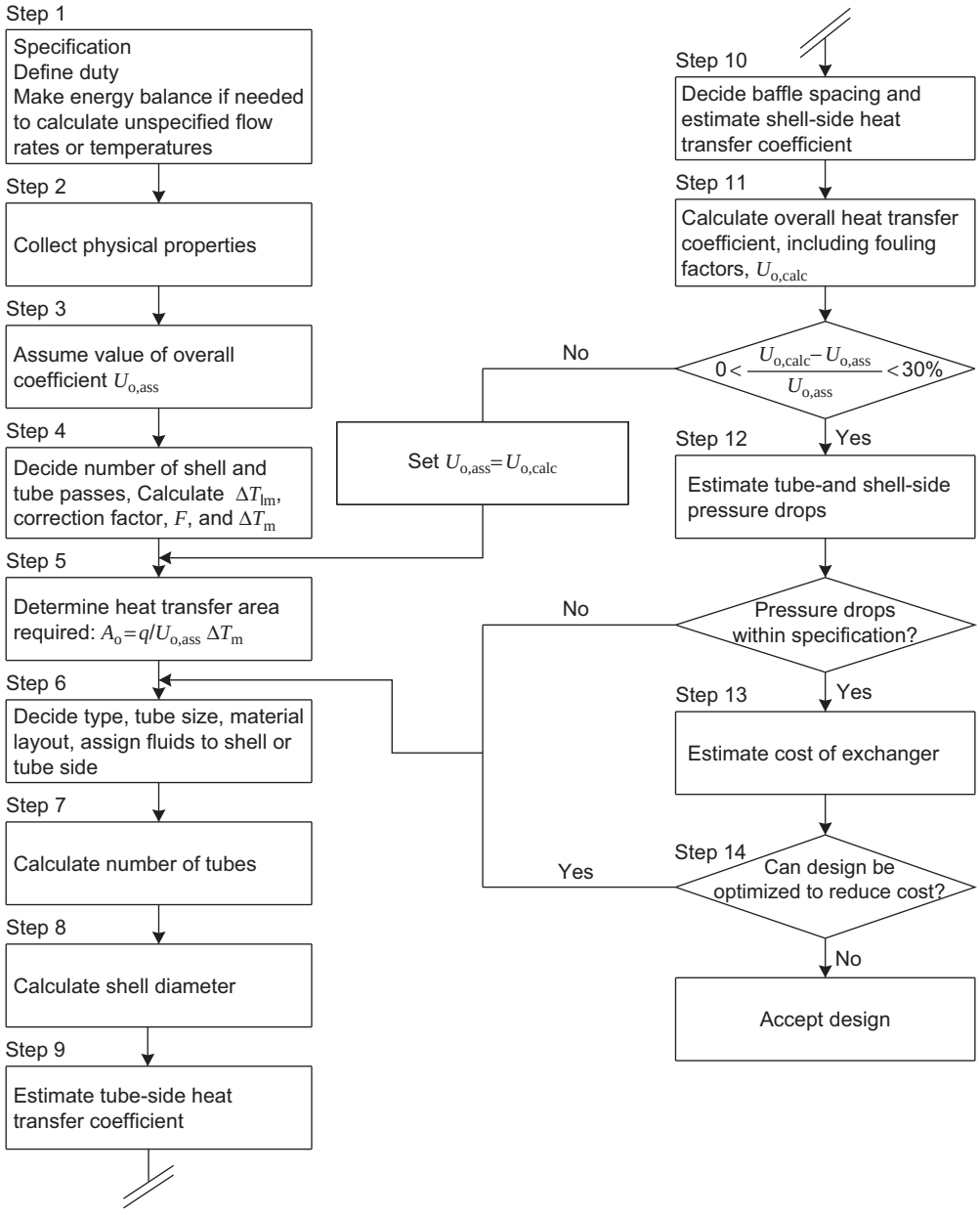


FIG. 19.31 Design procedure for shell and tube heat exchangers. *Example 19.2 and Fig. 19.31 were developed by the author for the Open University Course T333* Principles and Applications of Heat Transfer. *They are reproduced here by permission of the Open University.*

An energy balance gives:

$$\frac{7000}{3600} \times 2.01\,(t_2 - 40) = 1509.4$$

$t_2 = 78.6$ °C and the stream mean temperature $= (40 + 78.6)/2 = 59.3$ °C.

The specific heat at this temperature is 2.05 kJ/kg°C. A second trial calculation using this value gives $t_2 = 77.9$ °C and a new mean temperature of 58.9 °C. There is no significant change in the specific heat at this mean temperature from the value used, so take the crude stream outlet temperature to be 77.9 °C, say 78 °C.

Step 2: Physical properties

Kerosene	**Inlet**	**Mean**	**Outlet**	
Temperature	200	145	90	°C
Specific heat	2.72	2.47	2.26	kJ/kg°C
Thermal conductivity	0.130	0.132	0.135	W/m°C
Density	690	730	770	kg/m^3
Viscosity	0.22	0.43	0.80	mN sm^{-2}

Crude oil	Outlet	Mean	Inlet	
Temperature	78	59	40	°C
Specific heat	2.09	2.05	2.01	kJ/kg°C
Thermal conductivity	0.133	0.134	0.135	W/m°C
Density	800	820	840	kg/m^3
Viscosity	2.4	3.2	4.3	$mN\ sm^{-2}$

Step 3: Overall coefficient

For an exchanger of this type, the overall coefficient will be in the range of 300 to 500 $W/m^{2\circ}C$ (see Fig. 19.1 and Table 19.1), so start with 300 $W/m^{2\circ}C$.

Step 4: Exchanger type and dimensions

An even number of tube passes is usually the preferred arrangement, as this positions the inlet and outlet nozzles at the same end of the exchanger, which simplifies the pipework.

Start with one shell pass and two tube passes:

$$\Delta T_{l\ m} = \frac{(200-78)-(90-40)}{\ln\dfrac{(200-78)}{(90-40)}} = 80.7^{\circ}C \tag{19.4}$$

$$R = \frac{(200-90)}{(90-40)} = 2.9 \tag{19.6}$$

$$S = \frac{(78-40)}{(200-40)} = 0.24 \tag{19.7}$$

From Fig. 19.19, $F_t = 0.88$, which is acceptable.

So,

$$\Delta T_m = 0.88 \times 80.7 = 71.0^{\circ}C$$

Step 5: Heat transfer area

$$A_o = \frac{1509.4 \times 10^3}{300 \times 71.0} = 70.86\ m^2 \tag{19.1}$$

Step 6: Layout and tube size

Use a split-ring floating-head exchanger for efficiency and ease of cleaning. Neither fluid is corrosive and the operating pressure is not high, so a plain carbon steel can be used for the shell and tubes. The crude is dirtier than the kerosene, so put the crude through the tubes and the kerosene in the shell.

Use 19.05 mm (¾ inch) outside diameter, 14.83 mm inside diameter, 5 m long tubes (a popular size) on a triangular 23.81 mm pitch (pitch/dia. = 1.25).

Step 7: Number of tubes

Area of one tube (neglecting thickness of tubesheets):

$$= \pi \times 19.05 \times 10^{-3} \times 5 = 0.2992\ m^2$$

Number of tubes = 70.89/0.2992 = 237, say 240

So, for two passes, tubes per pass = 120

Check the tube-side velocity at this stage to see if it looks reasonable:

$$\text{Tube cross} - \text{sectional area} = \frac{\pi}{4}\left(14.83 \times 10^{-3}\right)^2 = 0.0001727\ m^2$$

$$\text{So area per pass} = 120 \times 0.0001727 = 0.02073\ m^2$$

$$\text{Volumetric flow} = \frac{70,000}{3600} \times \frac{1}{820} = 0.0237\ m^3/s$$

$$\text{Tube} - \text{side velocity, } u_t = \frac{0.0237}{0.02073} = 1.14\ m/s$$

The velocity is satisfactory, between 1 and 2 m/s, but may be a little low. This will show up when the pressure drop is calculated.

Step 8: Bundle and shell diameter

From Table 19.4, for two tube passes, $K_1 = 0.249$, $n_1 = 2.207$,
so,

$$D_b = 19.05\left(\frac{240}{0.249}\right)^{1/2.207} = 428 \text{ mm } (0.43 \text{ m}) \tag{19.3b}$$

For a split-ring floating-head exchanger, the typical shell clearance from Fig. 19.10 is 56 mm, so the shell inside diameter is:

$$D_s = 428 + 56 = 484 \text{ mm}$$

Step 9: Tube-side heat transfer coefficient

$$\text{Re} = \frac{\rho u d_i}{\mu} = \frac{820 \times 1.14 \times 14.83 \times 10^{-3}}{3.2 \times 10^{-3}} = 4332$$

$$\text{Pr} = \frac{C_p \mu}{k_f} = \frac{2.05 \times 10^3 \times 3.2 \times 10^{-3}}{0.134} = 48.96$$

$$\frac{L}{d_i} = \frac{5000}{14.83} = 337$$

From Fig. 19.23,

$$j_h = 3.2 \times 10^{-3}$$

$$\text{Nu} = 3.2 \times 10^{-3}(4332)(48.96)^{0.33} = 50.06 \tag{19.15}$$

$$h_i = 50.06\left(\frac{0.134}{14.83 \times 10^{-3}}\right) = 452 \text{ W/m}^{2\circ}\text{C}$$

This is clearly too low if U_o is to be 300 W/m$^{2\circ}$C. The tube-side velocity did look low, so increase the number of tube passes to four. This will halve the cross-sectional area in each pass and double the velocity.

$$\text{New } u_t = 2 \times 1.14 = 2.3 \text{ m/s}$$

$$\text{and Re} = 2 \times 4332 = 8664$$

$$j_h = 3.8 \times 10^{-3}$$

$$h_i = \left(\frac{0.134}{14.83 \times 10^{-3}}\right) \times 3.8 \times 10^{-3}\,(8664)(48.96)^{0.33}$$
$$= 1074 \text{ W/m}^{2\circ}\text{C}$$

Step 10: Shell-side heat transfer coefficient

Kern's method will be used. With four tube passes, the shell diameter will be larger than that calculated for two passes. For four passes $K_1 = 0.175$ and $n_1 = 2.285$.

$$D_b = 19.05\left(\frac{240}{0.175}\right)^{1/2.285} = 450 \text{ mm}, \quad (0.45 \text{ m}) \tag{19.3b}$$

The bundle to shell clearance is still around 56 mm, giving:

$$D_s = 506 \text{ mm} (\text{about } 20 \text{ inches})$$

As a first trial take the baffle spacing = $D_s/5$, say 100 mm. This spacing should give good heat transfer without too high a pressure drop.

$$A_s = \frac{(23.81 - 19.05)}{23.81} 506 \times 100 = 10,116 \text{ mm}^2 = 0.01012 \text{ m}^2 \tag{19.21}$$

$$d_e = \frac{1.10}{19.05}\left(23.81^2 - 0.917 \times 19.05^2\right) = 13.52 \text{ mm} \tag{19.23}$$

$$\text{Volumetric flow} - \text{rate on shell} - \text{side} = \frac{20,000}{3600} \times \frac{1}{730} = 0.0076 \ \text{m}^3/\text{s}$$

$$\text{Shell} - \text{side velocity} = \frac{0.0076}{0.01012} = 0.75 \ \text{m/s}$$

$$\text{Re} = \frac{730 \times 0.75 \times 13.52 \times 10^{-3}}{0.43 \times 10^{-3}} = 17,214$$

$$\text{Pr} = \frac{2.47 \times 10^3 \times 0.43 \times 10^{-3}}{0.132} = 8.05$$

Use segmental baffles with a 25% cut. This should give a reasonable heat transfer coefficient without too large a pressure drop.

From Fig. 19.29, $j_h = 4.52 \times 10^{-3}$.

Neglecting the viscosity correction:

$$h_s = \left(\frac{0.132}{13.52} \times 10^3\right) \times 4.52 \times 10^{-3} \times 17,214 \times 8.05^{0.33} = 1505 \ \text{W/m}^{2\circ}\text{C} \tag{19.25}$$

Step 11: Overall coefficient

$$\frac{1}{U_o} = \left(\frac{1}{1074} + 0.00035\right) \frac{19.05}{14.83} + \frac{19.05 \times 10^{-3} \text{Ln}\left(\frac{19.05}{14.83}\right)}{2 \times 55} + \frac{1}{1505} + 0.0002 \tag{19.2}$$

$$U_o = 386 \ \text{W/m}^{2\circ}\text{C}$$

This is above the initial estimate of 300 W/m$^{2\circ}$C. The number of tubes could possibly be reduced, but first check the pressure drops.

Step 12: Pressure drop: Tube side

240 tubes, four passes, tube i.d. 14.83 mm, u_t 2.3 m/s,

Re $= 8.7 \times 10^3$. From Fig. 19.24, $j_f = 5 \times 10^{-3}$.

$$\begin{aligned} \Delta P_t &= 4 \left(8 \times 5 \times 10^{-3}\left(\frac{5000}{14.83}\right) + 2.5\right) \frac{(820 \times 2.3^2)}{2} \\ &= 4(13.5 + 2.5)\frac{(820 \times 2.3^2)}{2} \\ &= 138,810 \ \text{N/m}^2, \ 1.4 \ \text{bar} \end{aligned} \tag{19.20}$$

This exceeds the specification. Return to step 6 and modify the design.

Modified design

The tube velocity needs to be reduced. This will reduce the heat transfer coefficient, so the number of tubes must be increased to compensate. There will also be a pressure drop across the inlet and outlet nozzles. Allow 0.1 bar for this, a typical figure (about 15% of the total), which leaves 0.7 bar across the tubes. Pressure drop is roughly proportional to the square of the velocity, and u_t is proportional to the number of tubes per pass. So the pressure drop calculated for 240 tubes can be used to estimate the number of tubes required.

Tubes needed $= 240/(0.6/1.4)^{0.5} = 365$

Say, 360 with four passes.

Retain four passes, as the heat transfer coefficient will be too low with two passes.

Second trial design: 360 tubes 19.05 mm o.d., 14.83 mm i.d., 5 m long, triangular pitch 23.81 mm.

$$D_b = 19.05\left(\frac{360}{0.175}\right)^{1/2.285} = 537 \ \text{mm}, \ (0.54 \ \text{m}) \tag{19.3b}$$

From Fig. 19.10, clearance with this bundle diameter = 59 mm:

$$D_s = 537 + 59 = 596 \text{ mm}$$

$$\text{Cross-sectional area per pass} = \frac{360}{4}\left(14.83 \times 10^{-3}\right)^2 \frac{\pi}{4} = 0.01555 \text{ m}^2$$

$$\text{Tube velocity, } u_t = \frac{0.02337}{0.01555} = 1.524 \text{ m/s}$$

$$\text{Re} = \frac{820 \times 1.524 \times 14.83 \times 10^{-3}}{3.2 \times 10^{-3}} = 5792$$

L/d is the same as the first trial: 337, so:

$$j_h = 3.6 \times 10^{-3}$$

$$h_i = \left(\frac{0.134}{14.83} \times 10^{-3}\right) 3.6 \times 10^{-3} \times 5792 \times 48.96^{0.33} = 680 \text{ W/m}^{2\circ}\text{C} \tag{19.15}$$

This looks satisfactory, but check the pressure drop before doing the shell-side calculation.

$$j_f = 5.5 \times 10^{-3}$$

$$\Delta P_t = 4\left(8 \times 5.5 \times 10^{-3}\left(\frac{5000}{14.83}\right) + 2.5\right) \frac{(820 \times 1.524^2)}{2} = 66,029 \text{ N/m}^2, 0.66 \text{ bar} \tag{19.20}$$

Well within specification.

Keep the same baffle cut and spacing:

$$A_s = \frac{(23.81 - 19.05)}{23.81} 596 \times 100 = 11,915 \text{ mm}^2, \quad 0.01192 \text{ m}^2 \tag{19.21}$$

$$u_s = \frac{0.0076}{0.01193} = 0.638 \text{ m/s}$$

$$d_e = 13.52 \text{ mm, as before}$$

$$\text{Re} = \frac{730 \times 0.638 \times 13.52 \times 10^{-3}}{0.43 \times 10^{-3}} = 14,644$$

$$\text{Pr} = 8.05$$

$$j_h = 4.8 \times 10^{-3}, \; j_f = 4.6 \times 10^{-2}$$

$$h_s = \left(\frac{0.132}{13.52 \times 10^{-3}}\right) 4.8 \times 10^{-3} \times 14,644 \times (8.05)^{0.33} = 1366 \text{ W/m}^{2\circ}\text{C, looks OK} \tag{19.25}$$

$$\Delta P_s = 8 \times 4.6 \times 10^{-2}\left(\frac{596}{13.52}\right)\left(\frac{5000}{100}\right)\frac{(730 \times 0.638^2)}{2} = 120,510 \text{ N/m}^2, \; 1.2 \text{ bar} \tag{19.26}$$

Too high; the specification only allowed 0.8 overall, including the loss over the nozzles. Check the overall coefficient to see if there is room to modify the shell-side design.

$$\frac{1}{U_o} = \left(\frac{1}{683} + 0.00035\right)\frac{19.05}{14.83} + \frac{19.05 \times 10^{-3} \ln\left(\frac{19.05}{14.88}\right)}{2 \times 55} + \frac{1}{1366} + 0.0002$$

$$U_o = 302 \text{ W/m}^{2\circ}\text{C} \tag{19.2}$$

$$U_o \text{ required} = \frac{Q}{(A_o \Delta T_{\text{lm}})}, \quad A_o = 360 \times 0.2992 = 107.7 \text{ m}^2,$$

$$\text{so } U_o \text{ required} = \frac{1509.4 \times 10^3}{(107.7 \times 71)} = 197 \text{ W/m}^{2\circ}\text{C}$$

The estimated overall coefficient is well above that required for design, 302 compared with 192 W/m$^{2\circ}$C, which gives scope for reducing the shell-side pressure drop.

Allow a drop of 0.1 bar for the shell inlet and outlet nozzles, leaving 0.7 bar for the shell-side flow. So, to keep within the specification, the shell-side velocity will have to be reduced by around $\sqrt{(1/2)} = 0.707$. To achieve this, the baffle spacing will need to be increased to $100/0.707 = 141$, say 140 mm.

$$A_s = \frac{(23.81 - 19.05)}{23.81} 596 \times 140 = 6881 \ \text{mm}^2, \ 0.167 \ \text{m}^2$$
$$u_s = \frac{0.0076}{0.0167} = 0.455 \ \text{m/s}, \tag{19.21}$$

Giving: Re = 10,443, $h_s = 1177$ W/m^2°C, $\Delta P_s = 0.47$ bar, and $U_o = 288$ W/m^2°C.

The pressure drop is now well within the specification.

Step 13: Estimate cost

The cost of this design can be estimated using the methods given in Chapter 7.

Step 14: Optimization

There is scope for optimizing the design by reducing the number of tubes, as the pressure drops are well within specification and the overall coefficient is well above that needed; however, the method used for estimating the coefficient and pressure drop on the shell side (Kern's method) is not accurate, so keeping to this design will give some margin of safety.

Viscosity correction factor

The viscosity correction factor $(\mu/\mu_w)^{0.14}$ was neglected when calculating the heat transfer coefficients and pressure drops. This is reasonable for the kerosene, as it has a relatively low viscosity, but it is not so obvious so for the crude oil. So, before firming up the design, the effect of this factor on the tube-side coefficient and pressure drop will be checked.

First, an estimate of the temperature at the tube wall, t_w is needed.

$$\text{The inside area of the tubes} = \pi \times 14.83 \times 10^{-3} \times 5 \times 360 = 83.86 \ \text{m}^2$$
$$\text{Heat flux} = Q/A = 1509.4 \times 10^3/83.86 = 17,999 \ \text{W/m}^2$$

As a rough approximation:

$$(t_w - t)h_i = 17,999$$

where t is the mean bulk fluid temperature = 59 °C.

$$\text{So,} \quad t_w = \frac{17,999}{680} + 59 = 86°\text{C}.$$

The crude oil viscosity at this temperature = 2.1×10^{-3} Ns/m^2.

$$\text{Giving} \left(\frac{\mu}{\mu_w}\right)^{0.14} = \left(\frac{3.2 \times 10^{-3}}{2.1 \times 10^{-3}}\right)^{0.14} = 1.06$$

Only a small factor, so the decision to neglect it was justified. Applying the correction would increase the estimated heat transfer coefficient, which is in the right direction. It would give a slight decrease in the estimated pressure drop.

Summary: The proposed design

Split ring, floating head, one shell pass, four tube passes.
360 carbon steel tubes, 5 m long, 19.05 mm o.d., 14.83 mm i.d., triangular pitch, pitch 23.18 mm.
Heat transfer area 107.7 m^2 (based on outside diameter).
Shell i.d. 597 mm (600 mm), baffle spacing 140 mm, 25% cut.
Tube-side coefficient 680 W/m^2°C, clean.
Shell-side coefficient 1366 W/m^2°C, clean.
Overall coefficient, estimated 288 W/m^2°C, dirty.
Overall coefficient required 197 W/m^2°C, dirty.
Dirt/fouling factors:
- Tube-side (crude oil) 0.00035 (W/m^2°C)$^{-1}$.
- Shell-side (kerosene) 0.0002 (W/m^2°C)$^{-1}$.

Pressure drops:
- Tube side, estimated 0.40 bar, +0.1 for nozzles; specified 0.8 bar overall.
- Shell side, estimated 0.45 bar, +0.1 for nozzles; specified 0.8 bar overall.

19.9.4 Commercial software for heat exchanger design

Computer methods for detailed design of heat exchangers are available in most of the commercial process simulation programs introduced in Chapter 4; see Table 4.1. For example, Aspen Technology's Aspen Engineering Suite contains the HTFS TASC program, and Honeywell's UniSim Design Suite can be linked to Honeywell's UniSim Heat Exchanger program, which is also based on the HTFS methods. The methods developed by HTRI can be licensed from them (www.HTRI.net).

All of the commercial heat exchanger design programs allow the user to upload process data and stream properties from a process simulation. Some care is needed when uploading data for streams that undergo partial vaporization or have other effects that cause a significant variation in heat capacity or other properties across the exchanger. When there are significant changes in fluid properties between the exchanger inlet and outlet, the designer should break the exchanger into several exchangers in series in the process simulation so as to obtain several sets of property data at intermediate temperatures for input into the heat exchanger software.

The details of running the commercial heat exchanger design programs are not addressed here, as each program is slightly different from the others; consult the user manuals and online help. The heat exchanger programs have both rating and design capability. They can be configured to determine a least cost design for given desired outlet temperatures and allowable pressure drop or to calculate the outlet stream temperatures and pressures given details of the exchanger geometry and process fluid inlet conditions. All of the programs allow the user to make quick adjustments to exchanger geometry and then recalculate to see the impact on the stream outlet temperatures and pressure drops.

Example 19.4

Optimize the design of Example 19.3 using commercial heat exchanger design software.

Solution

This problem was solved using UniSim Design Heat Exchanger.

Figs. 19.32 and 19.33 show the stream data and physical properties. The program was then run with the objective function set to minimum cost, giving the output shown in Fig. 19.34 and the setting plan shown in Fig. 19.35.

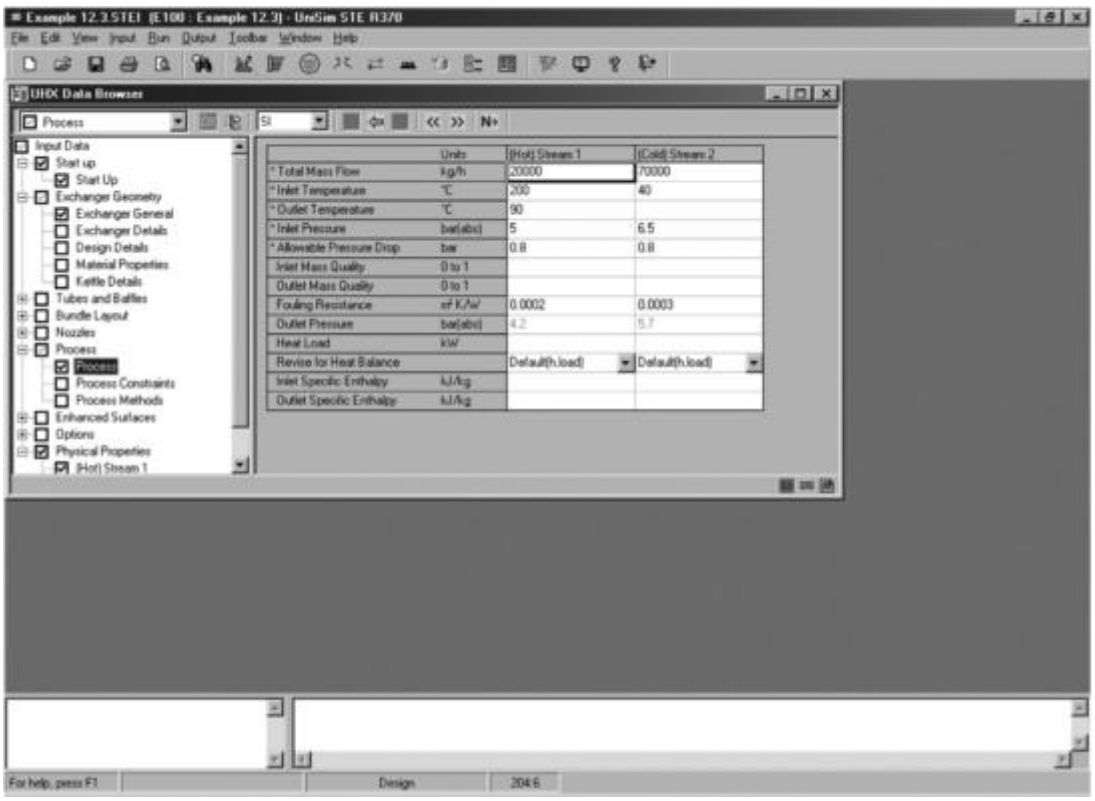


FIG. 19.32 Stream data for Example 19.4.

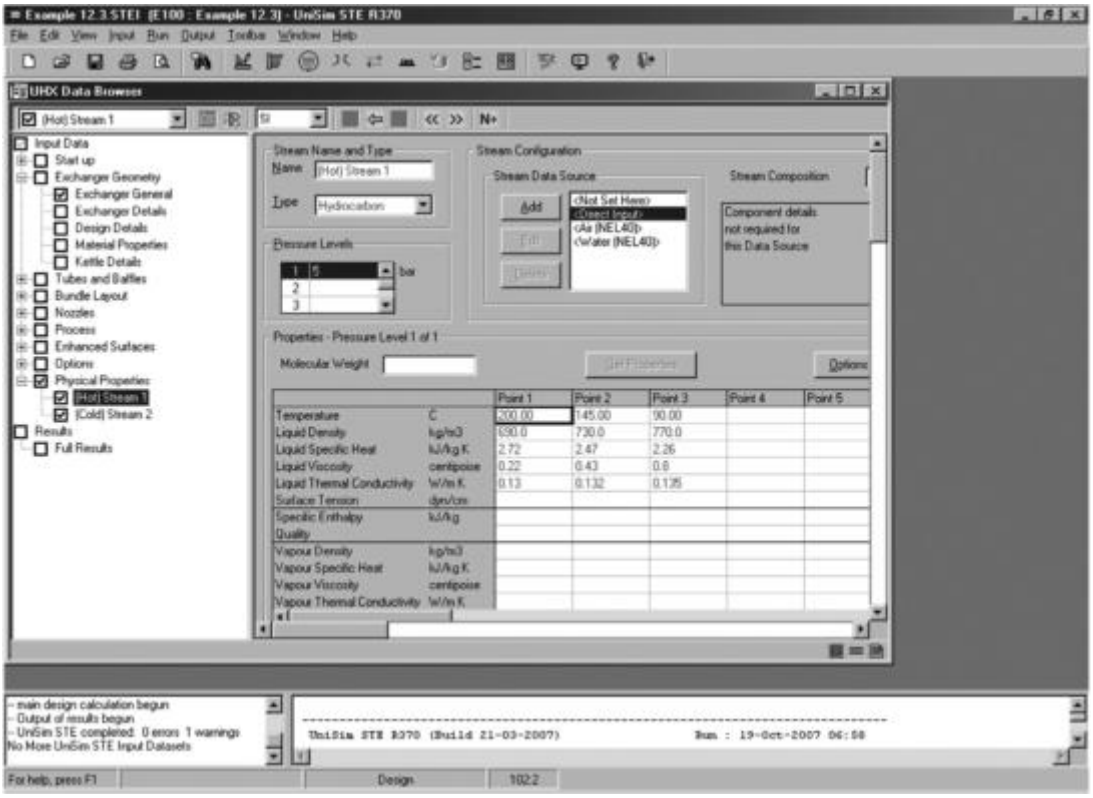


FIG. 19.33 Stream physical properties for Example 19.4.

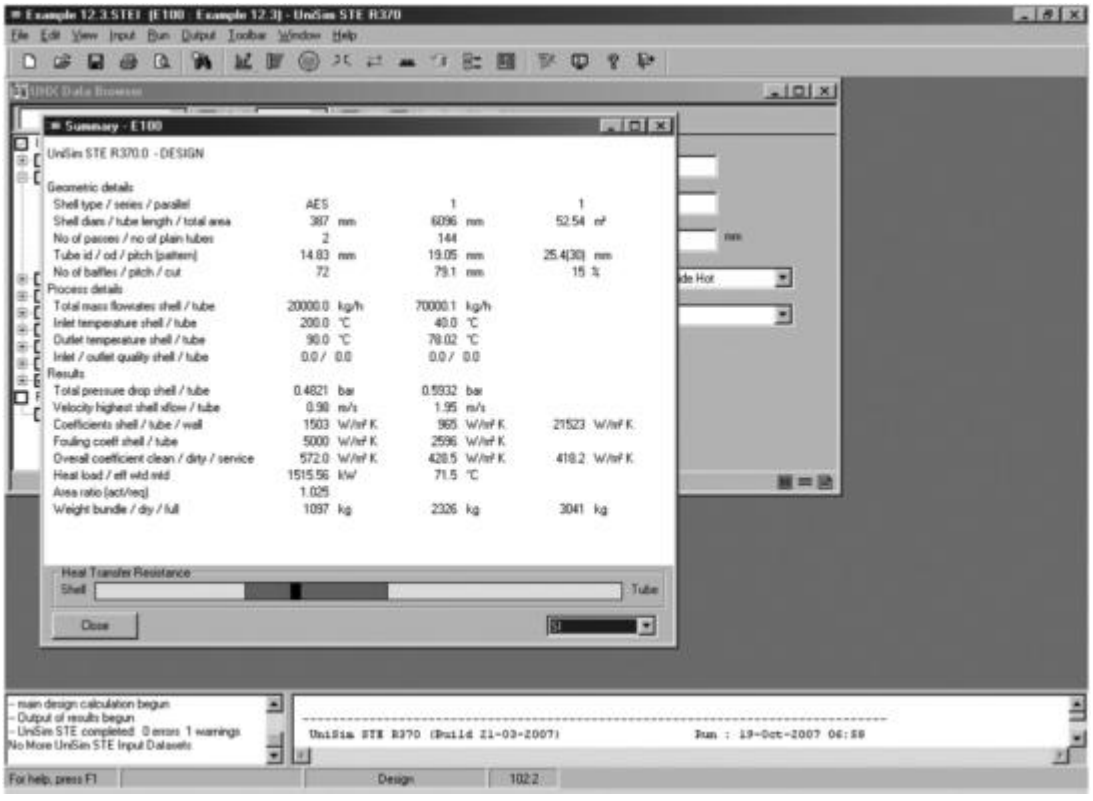
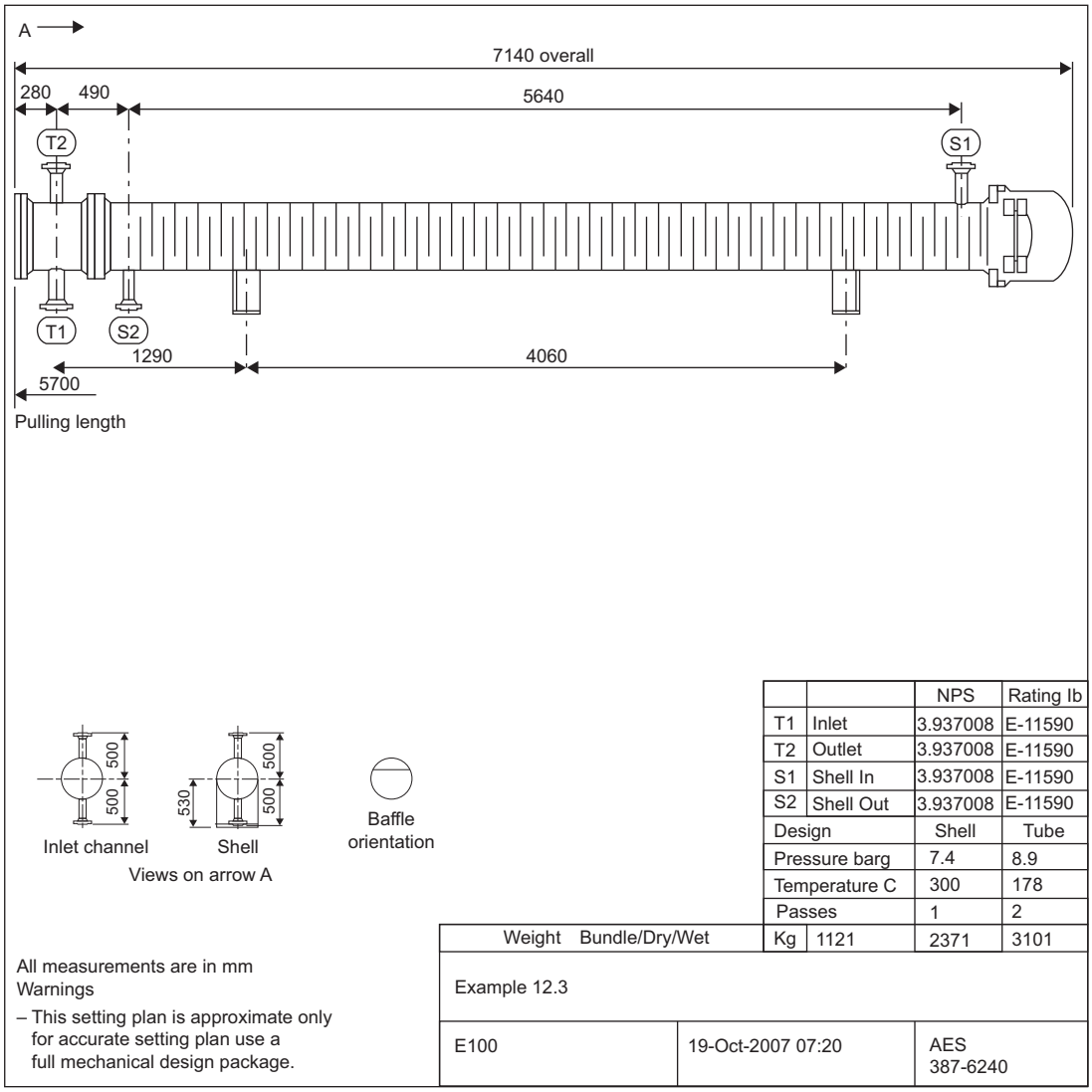


FIG. 19.34 UniSim Design STE (HTFS) program output.



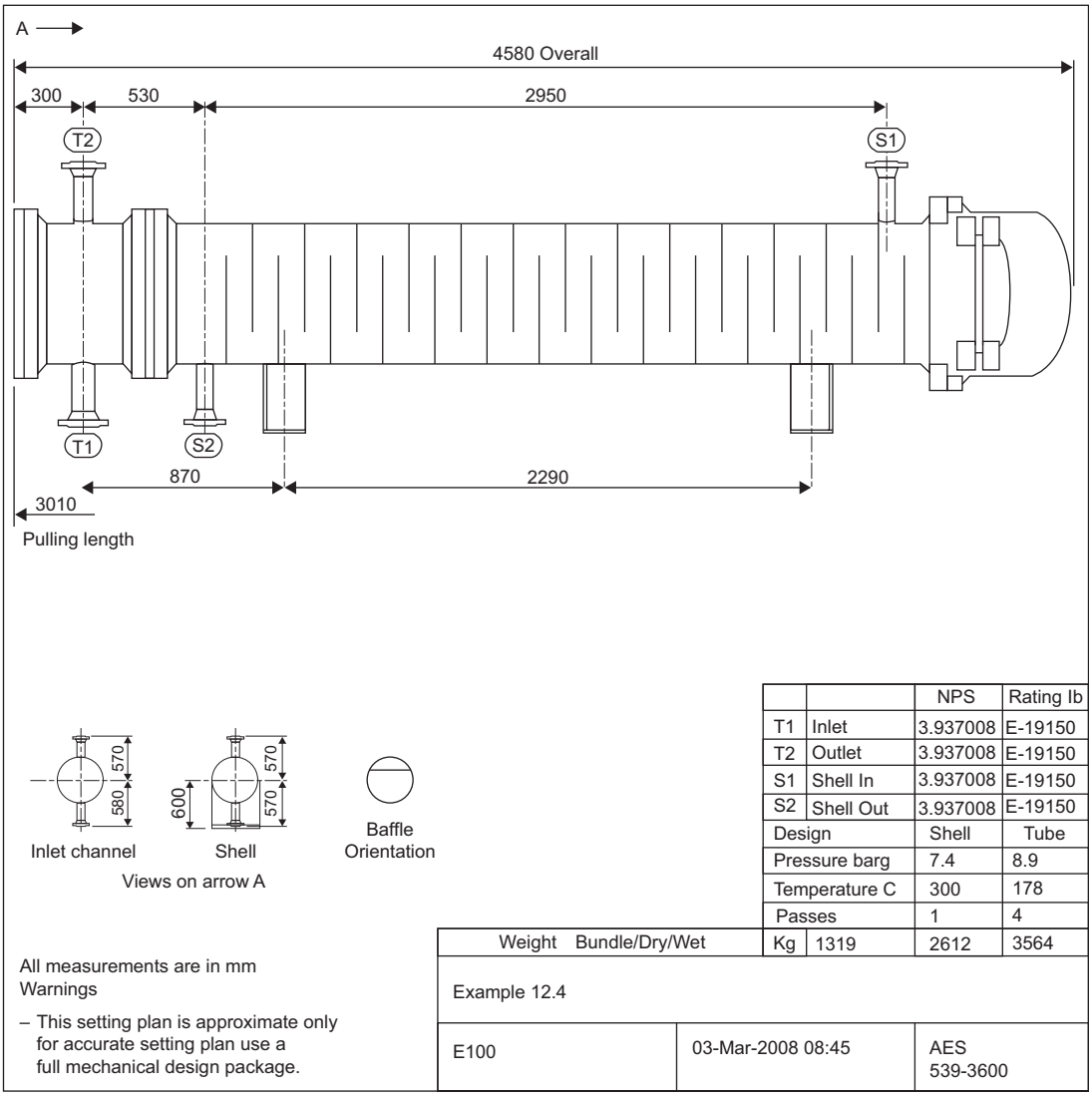
		NPS	Rating lb
T1	Inlet	3.937008	E-11590
T2	Outlet	3.937008	E-11590
S1	Shell In	3.937008	E-11590
S2	Shell Out	3.937008	E-11590
Design		Shell	Tube
Pressure barg		7.4	8.9
Temperature C		300	178
Passes		1	2
Weight Bundle/Dry/Wet	Kg	1121	2371	3101

FIG. 19.35 HTFS setting plan.

The program selected two tube passes with 6096 mm (20 ft) long tubes and many baffles (72) to obtain good countercurrent flow on the shell side. This design could cause problems with plot space, or with supporting the shell, or with withdrawing the bundle for cleaning and maintenance. The program was run again with the tube length constrained to be less than 4880 mm (16 ft). This gives a more compact design with four tube passes, 12-ft-tubes, and only 28 baffles, shown in Fig. 19.36.

The program initially gives a warning: "At some point(s) the cross flow fraction in the shell side flow model was less than 30%. This is below the expected range of values and may give poor heat transfer," When the baffle-to-shell and tube-to-baffle tolerances are specified using the values given in Section 19.5.7 (1.6 mm and 0.8 mm, respectively), then the design converges with no warnings. The TEMA sheet for the resulting design is given in Fig. 19.37.

Note that the more compact design did not make as good use of the allowable pressure drop on the shell side and also has a higher bundle weight and area, corresponding to a higher capital cost than the 20-ft-long exchanger initially designed. Note also that both designs developed using the HTFS software need substantially less area than the 107.7 m^2 predicted using Kern's method in Example 19.3.



		NPS	Rating lb
T1	Inlet	3.937008	E-19150
T2	Outlet	3.937008	E-19150
S1	Shell In	3.937008	E-19150
S2	Shell Out	3.937008	E-19150
Design		Shell	Tube
Pressure barg		7.4	8.9
Temperature C		300	178
Passes		1	4
Weight Bundle/Dry/Wet	Kg	1319	2612	3564

FIG. 19.36 Setting plan with length constrained.

19.10 Condensers

This section covers the design of shell and tube exchangers used as condensers. Direct contact condensers are discussed in Section 19.13.

The construction of a condenser is similar to other shell and tube exchangers, but with a wider baffle spacing, typically $l_B = D_s$.

Four condenser configurations are possible:

1. Horizontal, with condensation in the shell, and the cooling medium in the tubes.
2. Horizontal, with condensation in the tubes.
3. Vertical, with condensation in the shell.
4. Vertical, with condensation in the tubes.

Horizontal shell side and vertical tube side are the most commonly used types of condenser. A horizontal exchanger with condensation in the tubes is rarely used as a process condenser, but is the usual arrangement for heaters and vaporizers using condensing steam as the heating medium.

19.10.1 Heat transfer fundamentals

The fundamentals of condensation heat transfer are covered in Chhabra and Shankar (2017).

Heat exchager specification sheet

Customer												**Job No.**			
												Reference No.			
Address												**Proposal No.**			
Plant location												**Date**		**Rev.**	
Service of unit	Example 12.4											**Item No.**	E100		
Size	540–3600	**Type**	AES		Horizontal			**Connected**	1	**parallel**	1	**series**			
Surf./Unit (Gross)	65.71	m^2	**Shells/Unit**	1	**Surface/Shell (Gross)**	65.71	m^2								
Performance of one unit															
Fluid allocation			**Shell side**					**Tube side**							
Fluid name															
Fluid quantity,	**Total**	**kg/h**	20000.0					70000.2							
Vapour															
Liquid			20000.0		20000.0			70000.2		70000.2					
Steam															
Water															
Noncondensable															
Temperature (In/Out)		°C	200.0		90.0			40.0		78.0					
Density		kg/m^3	690.0		770.0			840.0		800.0					
Viscosity		**centipoise**	0.22		0.8			4.3		2.39925					
Molecular weight, vapour															
Molecular weight, Noncondensable															
Specific heat		**kJ/kg K**	2.72		2.26			2.01		2.09					
Thermal conductivity		**W/m K**	0.13		0.135			0.135		0.133					
Latent heat		**kJ/kg**													
Inlet pressure		**bar(abs)**	5.0					6.5							
Velocity		**m/s**	0.48					1.84							
Pressure drop, allow. / calc.		**bar**	0.8		0.14338			0.8		0.66002					
Fouling resistance (min.)		m^3 **K/W**	0.0002					0.0003 (0.00039 referred to OD)							
Heat exchaged	1515.56				**kW**	**MTD**	71.62	°C							
Transfer rate, service	345.3	**Dirty**	345.4	**Clean**	432.9	W/m^2 **K**									
Construction of one shell												**Sketch (bundle/nozzle orientation)**			
			Shell side		**Tube side**										
Design/test pressure	bar(g)		7.43		8.93										
Design temperature	°C		300.0		178.0										
No. passes per shell					4										
Corrosion allowance															
Connections	**In**		62.7		90.1										
Size &	**Out**		62.7		77.9										
Ratings	**Inter**														
Tube no.	305	**OD**	19.05	**mm**	**Thk**	2.11	**mm**	**Length**	3600	**mm**	**Pitch**	25.4	**mm**	**30deg**	
Tube type	**plain**							**Material**	Carbon steel						
Shell		**ID**	540	**OD**			**mm**	**Shell cover**						**(Integ.)(Remov.)**	
Channel or Bonnet	Carbon steel							**Channel cover**							
Tubesheet-stationary	Carbon steel							**Tubesheet-floating**							
Floating head cover								**Impingement protection**							
Baffles-cross	28	**Type**	Single segmental					**% Cut**	25.0	**Spacing c/c**	113.5	**Inlet**		**mm**	
Baffles-long								Seal type							
Supports-tube				**U-Bend**				**Type**							
Bypass seal arrangement								**Tube-Tubesheet joint**							
Expansion joint								**Type**							
ρV^2**-inlet nozzle**	4689.0			**Bundle entrance**	488.0			**Bundle exit**	437.3						
Gaskets	**Shell side**							**Tube side**							
	Floating head														
Code reuirements										**Tema class**	**R**				
Weight/shell	2612			**Filled with water**	3564			**Bundle**	1319					**kg**	
Remarks															

FIG. 19.37 TEMA specification sheet for Example 19.4.

The normal mechanism for heat transfer in commercial condensers is film-wise condensation. Drop-wise condensation will give higher heat transfer coefficients, but is unpredictable and is not yet considered a practical proposition for the design of condensers for general purposes.

The basic equations for film-wise condensation were derived by Nusselt (1916), and his equations form the basis for practical condenser design. The Nusselt equations are derived in Chhabra and Shankar (2017). In the Nusselt model of condensation, laminar flow is assumed in the film, and heat transfer is assumed to take place entirely by conduction through the film. In practical condensers, the Nusselt model will strictly only apply at low liquid and vapor rates and where the flowing condensate film is undisturbed. Turbulence can be induced in the liquid film at high liquid rates and by shear at high vapor rates. This will generally increase the rate of heat transfer

over that predicted using the Nusselt model. The effect of vapor shear and film turbulence are discussed in Chhabra and Shankar (2017); see also Butterworth (1978) and Taborek (1974).

Developments in the theory of condensation and their application in condenser design are reviewed by Owen and Lee (1983).

Physical properties

The physical properties of the condensate for use in the following equations are evaluated at the average condensate film temperature: the mean of the condensing temperature and the tube-wall temperature.

19.10.2 Condensation outside horizontal tubes

$$(h_c)_1 = 0.95 k_L \left[\frac{\rho_L(\rho_L - \rho_v)g}{\mu_L \Gamma}\right]^{1/3} \tag{19.27}$$

where $(h_c)_1$ = mean condensation film coefficient for a single tube, W/m^2°C
k_L = condensate thermal conductivity, W/m°C
ρ_L = condensate density, kg/m^3
ρ_v = vapor density, kg/m^3
μ_L = condensate viscosity, Ns/m^2
g = gravitational acceleration, 9.81 m/s^2
Γ = the tube loading, the condensate flow per unit length of tube, kg/m s

In a bank of tubes, the condensate from the upper rows of tubes will add to that condensing on the lower tubes. If there are N_r tubes in a vertical row and the condensate is assumed to flow smoothly from row to row (Fig. 19.38a) and if the flow remains laminar, the mean coefficient predicted by the Nusselt model is related to that for the top tube by:

$$(h_c)_{N_r} = (h_c)_1 N_r^{-1/4} \tag{19.28}$$

In practice, the condensate will not flow smoothly from tube to tube (see Fig. 19.38b) and the factor of $(N_r)^{-1/4}$ applied to the single tube coefficient in Equation 19.28 is considered to be too conservative. Based on results from commercial exchangers, Kern (1950) suggests using an index of 1/6. Frank (1978) suggests multiplying single tube coefficient by a factor of 0.75.

Using Kern's method, the mean coefficient for a tube bundle is given by:

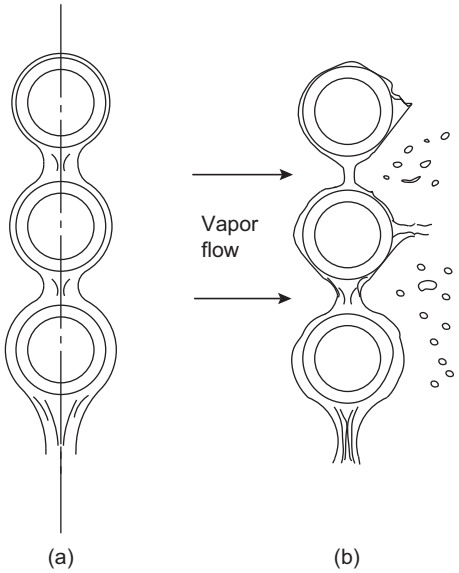


FIG. 19.38 Condensate flow over tube banks.

$$(h_c)_b = 0.95 k_L \left[\frac{\rho_L(\rho_L - \rho_v)g}{\mu_L \Gamma_h}\right]^{1/3} N_r^{-1/6} \tag{19.29}$$

where $\Gamma_h = \dfrac{W_c}{LN_t}$

and L = tube length,

W_c = total condensate flow,

N_t = total number of tubes in the bundle,

N_r = average number of tubes in a vertical tube row.

N_r can be taken as two-thirds of the number in the central tube row.

For low-viscosity condensates, the correction for the number of tube rows is generally ignored.

A procedure for estimating the shell-side heat transfer in horizontal condensers is given in the ESDU Design Guide, ESDU 84023.

19.10.3 Condensation inside and outside vertical tubes

For condensation inside and outside vertical tubes, the Nusselt model gives:

$$(h_c)_v = 0.926 k_L \left[\frac{\rho_L(\rho_L - \rho_v)g}{\mu_L \Gamma_v}\right]^{1/3} \tag{19.30}$$

where $(h_c)_v$ = mean condensation coefficient, W/m$^{2\circ}$C

Γ_v = vertical tube loading, condensate rate per unit tube perimeter, kg/m s for a tube bundle

$$\Gamma_v = \frac{W_c}{N_t \pi d_o} \quad \text{or} \quad \frac{W_c}{N_t \pi d_i}$$

Equation 19.30 will apply up to a Reynolds number of 30; above this value, waves on the condensate film become important. The Reynolds number for the condensate film is given by:

$$\mathrm{Re_c} = \frac{4\,\Gamma_v}{\mu_L}$$

The presence of waves will increase the heat transfer coefficient, so the use of Equation 19.30 above a Reynolds number of 30 will give conservative (safe) estimates. The effect of waves on condensate film on heat transfer is discussed by Kutateladze (1963).

Above a Reynolds number of around 2000, the condensate film becomes turbulent. The effect of turbulence in the condensate film was investigated by Colburn (1934), and Colburn's results are generally used for condenser design (Fig. 19.39). Equation 19.30 is also shown in Fig. 19.39. The Prandtl number for the condensate film is given by:

$$\mathrm{Pr_c} = \frac{C_p\,\mu_L}{k_L}$$

Fig. 19.39 can be used to estimate condensate film coefficients in the absence of appreciable vapor shear. Horizontal and downward vertical vapor flow will increase the rate of heat transfer, and the use of Fig. 19.39 will give conservative values for most practical condenser designs.

Boyko and Kruzhilin (1967) developed a correlation for shear-controlled condensation in tubes that is simple to use. Their correlation gives the mean coefficient between two points at which the vapor quality is known. The vapor quality x is the mass fraction of the vapor present. It is convenient to represent the Boyko–Kruzhilin correlation as:

$$(h_c)_{BK} = h'_t \left[\frac{J_1^{1/2} + J_2^{1/2}}{2}\right] \tag{19.31}$$

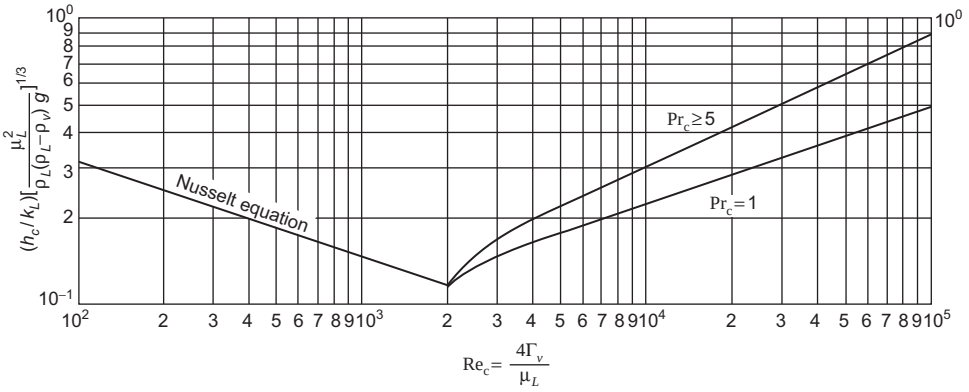


FIG. 19.39 Condensation coefficient for vertical tubes.

where

$$J = 1 + \left[\frac{\rho_L - \rho_v}{\rho_v}\right] x$$

and the suffixes 1 and 2 refer to the inlet and outlet conditions, respectively. h'_t is the tube-side coefficient evaluated for single-phase flow of the total condensate (the condensate at point 2). That is, the coefficient that would be obtained if the condensate filled the tube and was flowing alone; this can be evaluated using any suitable correlation for forced convection in tubes; see Section 19.8.

Boyko and Kruzhilin used the correlation:

$$h'_t = 0.021 \left(\frac{k_L}{d_i}\right) \mathrm{Re}^{0.8}\mathrm{Pr}^{0.43} \tag{19.32}$$

In a condenser, the inlet stream will normally be saturated vapor and the vapor will be totally condensed. For these conditions Equation 19.31 becomes:

$$(h_c)_{BK} = h'_t \left[\frac{1 + \sqrt{\rho_L/\rho_v}}{2}\right] \tag{19.33}$$

For the design of condensers with condensation inside the tubes and downward vapor flow, the coefficient should be evaluated using Fig. 19.39 and Equation 19.31 and the *higher* value selected.

Flooding in vertical tubes

When the vapor flows up the tube, which will be the usual arrangement for a reflux condenser, care must be taken to ensure that the tubes do not flood. Several correlations have been published for the prediction of flooding in vertical tubes; see Green and Southard (2018). One of the simplest to apply, which is suitable for use in the design of condensers handling low-viscosity condensates, is the criterion given by Hewitt and Hall-Taylor (1970); see also Butterworth (1977). Flooding should not occur if the following condition is satisfied:

$$\left[u_v^{1/2}\rho_v^{1/4} + u_L^{1/2}\rho_L^{1/4}\right] < 0.6[g d_i(\rho_L - \rho_v)]^{1/4} \tag{19.34}$$

where u_v and u_L are the velocities of the vapor and liquid based on each phase flowing in the tube alone and d_i is in meters. The critical condition will occur at the bottom of the tube, so the vapor and liquid velocities should be evaluated at this point.

Example 19.5

Estimate the heat transfer coefficient for steam condensing on the outside and on the inside of a 25 mm o.d., 21 mm i.d. vertical tube 3.66 m long. The steam condensate rate is 0.015 kg/s per tube, and condensation takes place at 3 bar. The steam will flow down the tube.

Solution

Physical properties, from steam tables:

$$\text{Saturation temperature} = 133.5^{\circ}\text{C}$$

$$\rho_L = 931 \text{ kg/m}^3$$

$$\rho_v = 1.65 \text{ kg/m}^3$$

$$k_L = 0.688 \text{ W/m}^{\circ}\text{C}$$

$$\mu_L = 0.21 \text{ mNs/m}^2$$

$$\text{Pr}_c = 1.27$$

Condensation outside the tube

$$\Gamma_v = \frac{0.015}{\pi \times 25 \times 10^{-3}} = 0.191 \text{ kg/s m}$$

$$\text{Re}_c = \frac{4 \times 0.191}{0.21 \times 10^{-3}} = 3638$$

From Fig. 19.39:

$$\frac{h_c}{k_L}\left[\frac{\mu_L^2}{\rho_L(\rho_L - \rho_v)g}\right]^{1/3} = 1.65 \times 10^{-1}$$

$$h_c = 1.65 \times 10^{-1} \times 0.688\left[\frac{(0.21 \times 10^{-3})^2}{931(931 - 1.65)9.81}\right]^{-1/3}$$

$$= \underline{\underline{6554 \text{ W/m}^{2\circ}\text{C}}}$$

Condensation inside the tube

$$\Gamma_v = \frac{0.015}{\pi \times 21 \times 10^{-3}} = 0.227 \text{ kg/s m}$$

$$\text{Re}_c = \frac{4 \times 0.227}{0.21 \times 10^{-3}} = 4324$$

From Fig. 19.39:

$$h_c = 1.72 \times 10^{-1} \times 0.688\left[\frac{(0.21 \times 10^{-3})^2}{931(931 - 1.65)9.81}\right]^{-1/3}$$

$$= 6832 \text{ W/m}^{2\circ}\text{C}$$

Using the Boyko–Kruzhilin method:

$$\text{Cross-sectional area of tube} = (21 \times 10^{-3})^2\frac{\pi}{4} = 3.46 \times 10^{-4} \text{ m}^2$$

Fluid velocity, total condensation:

$$u_t = \frac{0.015}{931 \times 3.46 \times 10^{-4}} = 0.047 \text{ m/s}$$

$$\text{Re} = \frac{\rho\, u\, d_i}{\mu} = \frac{931 \times 0.047 \times 21 \times 10^{-3}}{0.21 \times 10^{-3}} = 4376$$

$$h_t = 0.021 \times \frac{0.688}{21 \times 10^{-3}}(4376)^{0.8}(1.27)^{0.43} = 624 \text{ W/m}^{2\circ}\text{C} \tag{19.32}$$

$$h_c = 624\left[\frac{1+\sqrt{931/1.65}}{2}\right] = 7723 \text{ W/m}^{2\circ}\text{C} \tag{19.33}$$

Take higher value, $h_c = \underline{\underline{7723 \text{ W/m}^{2\circ}\text{C}}}$

Example 19.6

It is proposed to use an existing distillation column, which is fitted with a dephlegmator (reflux condenser) that has 200 vertical, 50 mm i.d. tubes for separating benzene from a mixture of chlorobenzenes. The top product will be 2500 kg/h benzene, and the column will operate with a reflux ratio of 3. Check if the tubes are likely to flood. The condenser pressure will be 1 bar.

Solution

The vapor will flow up and the liquid down the tubes. The maximum flow rates of both will occur at the base of the tube.

$$\text{Vapor flow} = (3+1) \times 2500 = 10,000 \text{ kg/h}$$

$$\text{Liquid flow} = 3 \times 2500 = 7,500 \text{ kg/h}$$

$$\text{Total area of tubes} = \frac{\pi}{4}\left(50 \times 10^{-3}\right)^2 \times 200 = 0.39 \text{ m}^2$$

Densities at benzene boiling point:

$$\rho_L = 840 \text{ kg/m}^3, \quad \rho_v = 2.7 \text{ kg/m}^3$$

Vapor velocity (vapor flowing alone in tube):

$$u_v = \frac{10,00}{3600 \times 0.39 \times 2.7} = 2.64 \text{ m/s}$$

Liquid velocity (liquid alone):

$$u_L = \frac{7500}{3600 \times 0.39 \times 840} = 0.006 \text{ m/s}$$

From Equation 19.34 for no flooding:

$$\left[u_v^{1/2}\rho_v^{1/4} + u_L^{1/2}\rho_L^{1/4}\right] < 0.6[g d_i(\rho_L - \rho_v)]^{1/4}$$

$$\left[(2.64)^{1/2}(2.7)^{1/4} + (0.006)^{1/2}(840)^{1/4}\right] < 0.6\left[9.81 \times 50 \times 10^{-3}(840 - 2.7)\right]^{1/4}$$

$$[2.50] < [2.70]$$

Tubes should not flood, but there is little margin of safety.

19.10.4 Condensation inside horizontal tubes

Where condensation occurs in a horizontal tube, the heat transfer coefficient at any point along the tube depends on the flow pattern at that point. The various patterns that can exist in two-phase flow are shown in Fig. 19.40 and are discussed in Chhabra and Shankar (2017). In condensation, the flow will vary from a single-phase vapor at the inlet to a single-phase liquid at the outlet, with all the possible patterns of flow occurring between these points. Bell et al. (1970) give a method for following the change in flow pattern as condensation occurs on a Baker flow-regime map. Correlations for estimating the average condensation coefficient have been published by several workers, but there is no generally satisfactory method that will give accurate predictions over a wide flow range. A comparison of the published methods is given by Bell et al. (1970).

Two flow models are used to estimate the mean condensation coefficient in horizontal tubes: stratified flow (Fig. 19.41a) and annular flow (see Fig. 19.41b). The stratified-flow model represents the limiting condition at low condensate and vapor rates, and the annular model the condition at high vapor and low condensate rates. For the stratified-flow model, the condensate film coefficient can be estimated from the Nusselt equation, applying a suitable correction for the reduction in the coefficient caused by the accumulation of condensate in the bottom of the tube. The correction factor will typically be around 0.8, so the coefficient for stratified flow can be estimated from:

$$(h_c)_s = 0.76 k_L \left[\frac{\rho_L(\rho_L - \rho_v)g}{\mu_L \Gamma_h}\right]^{1/3} \tag{19.35}$$

The Boyko–Kruzhilin equation, Equation 19.31, can be used to estimate the coefficient for annular flow.

For condenser design, the mean coefficient should be evaluated using the correlations for both annular and stratified flow and the *higher* value selected.

19.10.5 Condensation of steam

Steam is frequently used as a heating medium. The film coefficient for condensing steam can be calculated using the methods given in the previous sections, but as the coefficient will be high and will rarely be the limiting coefficient, it is customary to assume a typical conservative value for design purposes. For air-free steam, a coefficient of 8000 W/m^2°C (1500 Btu/h ft^2°F) can be used.

19.10.6 Mean temperature difference

A pure, saturated vapor will condense at a fixed temperature, at constant pressure. For an isothermal process such as this, the simple logarithmic mean temperature difference can be used in Equation 19.1; no correction factor for multiple passes is needed. The logarithmic mean temperature difference will be given by:

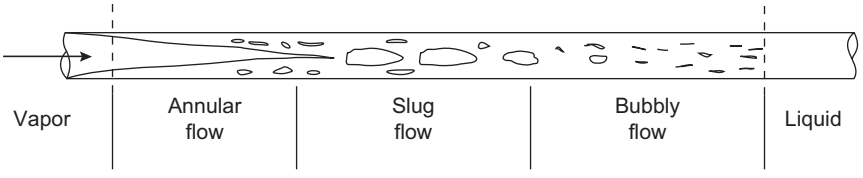


FIG. 19.40 Flow patterns, vapor condensing in a horizontal tube.

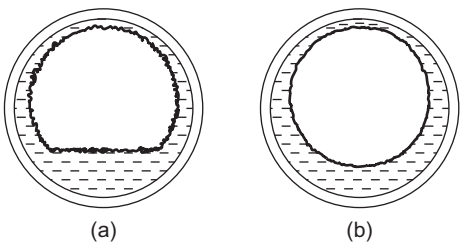


FIG. 19.41 Flow patterns in condensation. (a) Stratified flow. (b) Annular flow.

$$\Delta T_{lm} = \frac{(t_2 - t_1)}{\ln\left[\frac{T_{sat} - t_1}{T_{sat} - t_2}\right]} \tag{19.36}$$

where T_{sat} = saturation temperature of the vapor
t_1 = inlet coolant temperature
t_2 = outlet coolant temperature

When the condensation process is not exactly isothermal but the temperature change is small, such as where there is a significant change in pressure or where a narrow boiling range multicomponent mixture is being condensed, the logarithmic temperature difference can still be used, but the temperature correction factor will be needed for multipass condensers. The appropriate terminal temperatures should be used in the calculation.

19.10.7 Desuperheating and subcooling

When the vapor entering the condenser is superheated and the condensate leaving the condenser is cooled below its boiling point (subcooled), the temperature profile will be as shown in Fig. 19.42.

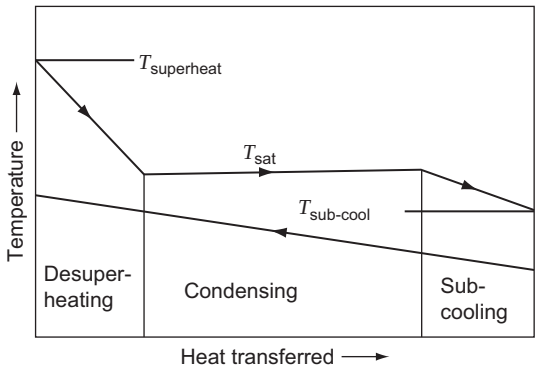


FIG. 19.42 Condensation with desuperheating and subcooling.

Desuperheating

If the degree of superheat is large, it will be necessary to divide the temperature profile into sections and determine the mean temperature difference and heat transfer coefficient separately for each section. If the tube wall temperature is below the dew point of the vapor, liquid will condense directly from the vapor onto the tubes. In these circumstances, it has been found that the heat transfer coefficient in the desuperheating section is close to the value for condensation and can be taken as the same. So, where the amount of superheat is not excessive, say less than 25% of the latent heat load, and the outlet coolant temperature is well below the vapor dew point, the sensible heat load for desuperheating can be lumped with the latent heat load. The total heat transfer area required can then be calculated using a mean temperature difference based on the saturation temperature (not the superheat temperature) and the estimated condensate film heat transfer coefficient.

Subcooling of condensate

Some subcooling of the condensate will usually be required to control the net positive suction head at the condensate pump (see Chapter 20) or to cool a product for storage. Where the amount of subcooling is large, it is more efficient to subcool in a separate exchanger. A small amount of subcooling can be obtained in a condenser by controlling the liquid level so that some part of the tube bundle is immersed in the condensate.

In a horizontal shell-side condenser, a dam baffle can be used (Fig. 19.43a). A vertical condenser can be operated with the liquid level above the bottom tubesheet (see Fig. 19.43b).

The temperature difference in the subcooled region will depend on the degree of mixing in the pool of condensate. The limiting conditions are plug flow and complete mixing. The temperature profile for plug flow is that shown in Fig. 19.42. If the pool is perfectly mixed, the condensate temperature will be constant over the subcooling region and equal to the condensate outlet temperature. Assuming perfect mixing will give a very conservative (safe) estimate of the mean temperature difference. As the liquid velocity will be low in the subcooled region, the heat transfer

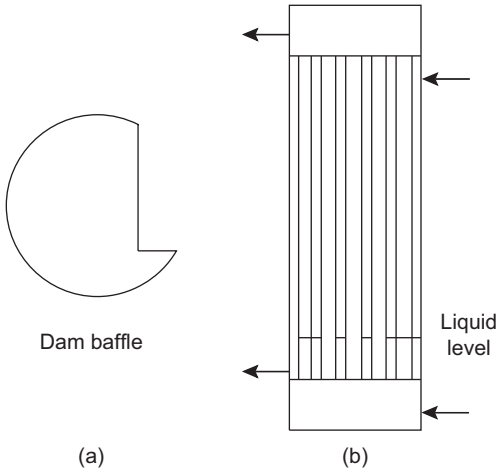


FIG. 19.43 Arrangements for subcooling.

coefficient should be estimated using correlations for natural convection (see Chhabra & Shankar 2017); a typical value would be 200 W/m$^{2\circ}$C.

19.10.8 Condensation of mixtures

The correlations given in the previous sections apply to the condensation of a single component, such as an essentially pure overhead product from a distillation column. The design of a condenser for a mixture of vapors is more difficult.

The term *"mixture of vapors"* covers three related situations of practical interest:

1. Total condensation of a multicomponent mixture, such as the overheads from a multicomponent distillation.
2. Condensation of only part of a multicomponent vapor mixture, all components of which are theoretically condensable. This situation will occur where the dew point of some of the lighter components is above the coolant temperature. The uncondensed component may be soluble in the condensed liquid, such as in the condensation of some hydrocarbon mixtures containing light "gaseous" components.
3. Condensation from a noncondensable gas, where the gas is not soluble to any extent in the liquid condensed. These exchangers are often called cooler-condensers.

The following features, common to all these situations, must be considered when developing design methods for mixed vapor condensers:

1. The condensation will not be isothermal. As the heavy component condenses out, the composition of the vapor, and therefore its dew point, changes.
2. Because the condensation is not isothermal, there will be a transfer of sensible heat from the vapor to cool the gas to the dew point. There will also be a transfer of sensible heat from the condensate, as it must be cooled from the temperature at which it condensed to the outlet temperature. The transfer of sensible heat from the vapor can be particularly significant, as the sensible heat transfer coefficient will be appreciably lower than the condensation coefficient.
3. As the composition of the vapor and liquid change throughout the condenser, their physical properties vary.
4. The heavy component must diffuse through the lighter components to reach the condensing surface. The rate of condensation will be governed by the rate of diffusion, as well as the rate of heat transfer.

Temperature profile

To evaluate the true temperature difference (driving force) in a mixed vapor condenser, a condensation curve (temperature vs. enthalpy diagram) must be calculated, showing the change in vapor temperature versus heat transferred throughout the condenser (Fig. 19.44). The temperature profile depends on the liquid-flow pattern in the condenser. There are two limiting conditions of condensate–vapor flow:

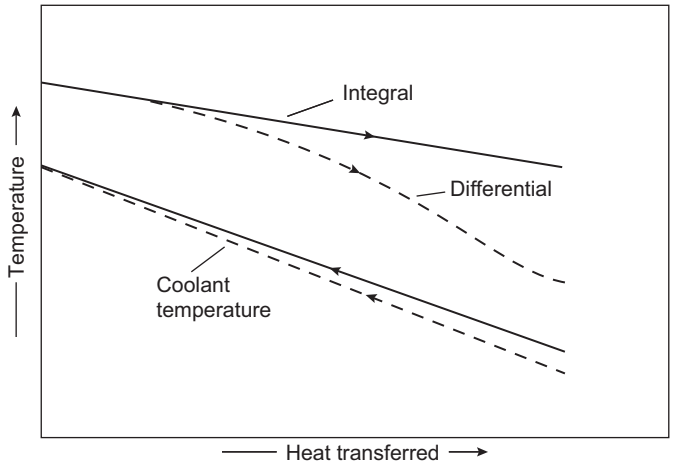


FIG. 19.44 Condensation curves.

1. Differential condensation, in which the liquid separates from the vapor from which it has condensed. This process is analogous to differential, or Rayleigh, distillation, and the condensation curve can be calculated using methods similar to those for determining the change in composition in differential distillation; see Chhabra and Gurappa (2019).
2. Integral condensation, in which the liquid remains in equilibrium with the uncondensed vapor. The condensation curve can be determined using procedures similar to those for multicomponent flash distillation given in Chapter 17. This will be a relatively simple calculation for a binary mixture, but complex and tedious for mixtures of more than two components.

It is normal practice to assume that integral condensation occurs. The conditions for integral condensation will be approached if condensation is carried out in one pass so that the liquid and vapor follow the same path as in a vertical condenser with condensation inside or outside the tubes. In a horizontal shell-side condenser, the condensate will tend to separate from the vapor. The mean temperature difference will be lower for differential condensation, and arrangements where liquid separation is likely to occur should generally be avoided for the condensation of mixed vapors.

Where integral condensation can be considered to occur, the use of a corrected logarithmic mean temperature difference based on the terminal temperatures will generally give a conservative (safe) estimate of the mean temperature difference that can be used in preliminary design calculations.

Estimation of heat transfer coefficients

Total condensation. For the design of a multicomponent condenser in which the vapor is totally condensed, an estimate of the mean condensing coefficient can be made using the single component correlations with the liquid physical properties evaluated at the average condensate composition. It is the usual practice to apply a factor of safety to allow for the sensible heat transfer and any resistance to mass transfer. Frank (1978) suggests a factor of 0.65, but this is probably too pessimistic. Kern (1950) suggests increasing the area calculated for condensation alone by the ratio of the total heat (condensing + sensible) to the condensing load. Where a more exact estimate of the coefficient is required and justified by the data, the rigorous methods developed for partial condensation can be used.

Partial condensation. The methods developed for partial condensation and condensation from a noncondensable gas can be divided into two classes:

1. Empirical methods: Approximate methods in which the resistance to heat transfer is considered to control the rate of condensation and the mass transfer resistance is neglected. Design methods have been published by Silver (1947), Bell and Ghaly (1973), and Ward (1960).
2. Analytical methods: More exact procedures that are based on some model of the heat and mass transfer process and which take into account the diffusion resistance to mass transfer. The classic method is that of Colburn and Hougen (1934); see also Colburn and Drew (1937) and Porter and Jeffreys (1963). The analytical methods are complex, requiring iterative calculations or graphical procedures. They are suited for computer solutions using

numerical methods, and proprietary design programs are available. Examples of the application of the Colburn and Drew method are given by Kern (1950) and Jeffreys (1961). The method is discussed briefly in Chhabra and Shankar (2017).

An assessment of the methods available for the design of condensers where the condensation is from a noncondensable gas is given by McNaught (1983).

Approximate methods. The local coefficient for heat transfer can be expressed in terms of the local condensate film coefficient h'_c and the local coefficient for sensible heat transfer from the vapor (the gas film coefficient) h'_g by a relationship first proposed by Silver (1947):

$$\frac{1}{h'_{cg}} = \frac{1}{h'_c} + \frac{Z}{h'_g} \tag{19.37}$$

where $h\prime_{cg}$= the local effective cooling-condensing coefficient

$$\text{and} \quad Z = \frac{\Delta H_s}{\Delta H_t} = xC_{pg}\frac{dT}{dH_t},$$

$(\Delta H_s/\Delta H_t)$ = the ratio of the change in sensible heat to the total enthalpy change
(dT/dH_t) = slope of the temperature−enthalpy curve
x = vapor quality, mass fraction of vapor
C_{pg} = vapor (gas) specific heat

The term dT/dH_t can be evaluated from the condensation curve, h'_c from the single component correlations, and h'_g from correlations for forced convection.

If this is done at several points along the condensation curve, the area required can be determined by graphical or numerical integration of the expression:

$$A = \int_0^{Q_t} \frac{dQ}{U\,(T_v - t_c)} \tag{19.38}$$

where Q_t = total heat transferred
U = overall heat transfer coefficient from Equation 19.1, using h'_{cg},
T_v = local vapor (gas) temperature
t_c = local cooling medium temperature

Gilmore (1963) gives an integrated form of Equation 19.37, which can be used for the approximate design of partial condensers:

$$\frac{1}{h_{cg}} = \frac{1}{h_c} + \frac{Q_g}{Q_t}\frac{1}{h_g} \tag{19.39}$$

where h_{cg} = mean effective coefficient
h_c = mean condensate film coefficient, evaluated from the single-component correlations at the average condensate composition and total condensate loading
h_g = mean gas film coefficient, evaluated using the average vapor flow rate: arithmetic mean of the inlet and outlet vapor (gas) flow rates
Q_g = total sensible heat transfer from vapor (gas)
Q_t = total heat transferred: latent heat of condensation + sensible heat for cooling the vapor (gas) and condensate

As a rough guide, the following rules of thumb suggested by Frank (1978) can be used to decide the design method to use for a partial condenser (cooler-condenser):

1. Noncondensables <0.5%: Use the methods for total condensation; ignore the presence of the uncondensed portion.
2. Noncondensables >70%: Assume the heat transfer is by forced convection only. Use the correlations for forced convection to calculate the heat transfer coefficient but include the latent heat of condensation in the total heat load transferred.
3. Between 0.5% and 70% noncondensables: Use methods that consider both mechanisms of heat transfer.

In partial condensation, it is usually better to put the condensing stream on the shell side and to select a baffle spacing that will maintain high vapor velocities, and therefore high sensible heat transfer coefficients.

Fog formation. In the condensation of a vapor from a noncondensable gas, if the bulk temperature of the gas falls below the dew point of the vapor, liquid can condense out directly as a mist or fog. This condition is undesirable, as liquid droplets may be carried out of the condenser. Fog formation in cooler-condensers is discussed by Colburn and Edison (1941) and LoPinto (1982). Steinmeyer (1972) gives criteria for the prediction of fog formation. Demisting pads can be used to separate entrained liquid droplets.

19.10.9 Pressure drop in condensers

The pressure drop on the condensing side is difficult to predict, as two phases are present and the vapor mass velocity is changing throughout the condenser.

A common practice is to calculate the pressure drop using the methods for single-phase flow and apply a factor to allow for the change in vapor velocity. For total condensation, Frank (1978) suggests taking the pressure drop as 40% of the value based on the inlet vapor conditions; Kern (1950) suggests a factor of 50%.

An alternative method, which can also be used to estimate the pressure drop in a partial condenser, is given by Gloyer (1970). The pressure drop is calculated using an average vapor flow rate in the shell (or tubes) estimated as a function of the ratio of the vapor flow rate in and out of the shell (or tubes) and the temperature profile.

$$W_s \text{ (average)} = W_s \text{ (inlet)} \times K_2 \tag{19.40}$$

K_2 is obtained from Fig. 19.45.

$\Delta T_{in}/\Delta T_{out}$ in Fig. 19.45 is the ratio of the terminal temperature differences.

These methods can be used to make a crude estimate of the likely pressure drop. A reliable prediction can be obtained by treating the problem as one of two-phase flow. For tube-side condensation, the general methods for two-phase flow in pipes can be used; see Collier and Thome (1994) and Chhabra and Shankar (2017). As the flow pattern will be changing throughout condensation, some form of step-wise procedure must be used. Two-phase flow on the shell side is discussed by Grant (1973), who gives a method for predicting the pressure drop based on Tinker's shell-side flow model. More sophisticated methods are available in the commercial heat exchanger design programs from HTFS and HTRI.

A method for estimating the pressure drop on the shell side of horizontal condensers is given in the ESDU Design Guide, ESDU 84023 (1985).

Pressure drop is only likely to be a major consideration in the design of vacuum condensers and where reflux is returned to a column by gravity flow from the condenser.

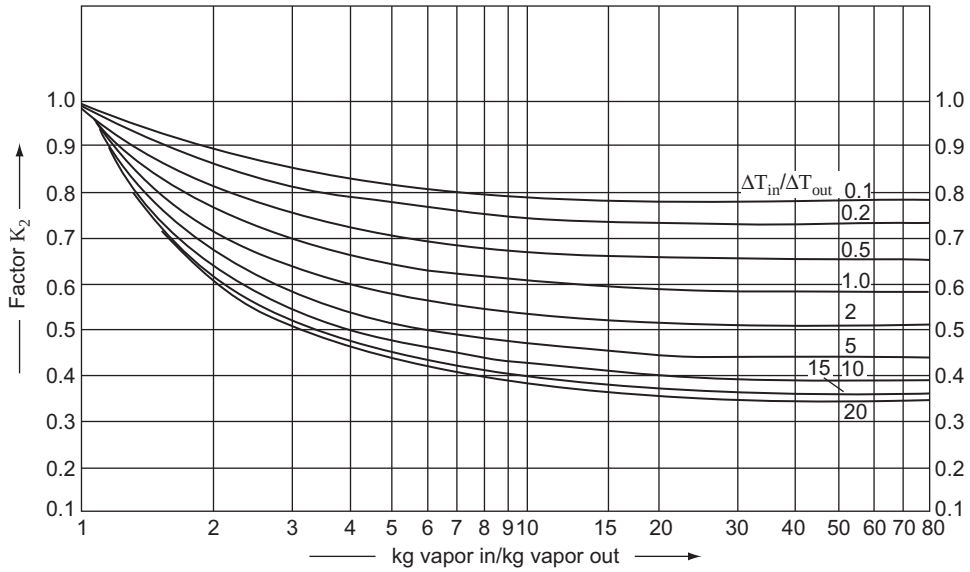


FIG. 19.45 Factor for average vapor flow rate for pressure-drop calculation.

Example 19.7

Design a condenser for the following duty: 45,000 kg/h of mixed light hydrocarbon vapors to be condensed. The condenser to operate at 10 bar. The vapor will enter the condenser saturated at 60 °C and the condensation will be complete at 45 °C. The average molecular weight of the vapors is 52. The enthalpy of the vapor is 596.5 kJ/kg and the condensate 247.0 kJ/kg. Cooling water is available at 30 °C, and the temperature rise is to be limited to 10 °C. Plant standards require tubes of 20 mm o.d., 16.8 mm i.d., 4.88 m (16 ft) long of admiralty brass. The vapors are to be totally condensed, and no subcooling is required.

Solution

Only the thermal design will be done. The physical properties of the mixture will be taken as the mean of those for n-propane (MW = 44) and n-butane (MW = 58) at the average temperature.

$$\text{Heat transferred from vapour} = \frac{45,000}{3600}(596.5 - 247.0) = 4368.8 \text{ kW}$$

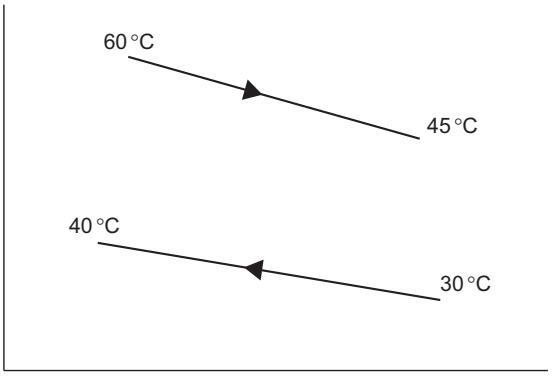
$$\text{Cooling water flow} = \frac{4368.8}{(40-30)4.18} = \underline{\underline{104.5 \text{ kg/s}}}$$

Assumed overall coefficient (Table 19.1) = 900 W/m^2°C.

Mean temperature difference: The condensation range is small and the change in saturation temperature will be linear, so the corrected logarithmic mean temperature difference can be used.

$$R = \frac{(60-45)}{(40-30)} = 1.5 \tag{19.6}$$

$$S = \frac{(40-30)}{(60-30)} = 0.33 \tag{19.7}$$



Try a horizontal exchanger, condensation in the shell, four tube passes. For one shell pass, four tube passes, from Fig. 19.19, $F_t = 0.92$:

$$\Delta T_{lm} = \frac{(60-40)-(45-30)}{\ln\frac{(60-40)}{(45-30)}} = 17.4°\text{C}$$

$$\Delta T_{lm} = 0.92 \times 17.4 = 16°\text{C}$$

$$\text{Trial area} = \frac{4368.8 \times 10^3}{900 \times 16} = 303 \text{ m}^2$$

$$\text{Surface area of one tube} = 20 \times 10^{-3}\pi \times 4.88 = 0.305 \text{ m}^2 \text{(ignore tubesheet thickness)}$$

$$\text{Number of tubes} = \frac{303}{0.305} = 992$$

Use square pitch, $P_t = 1.25 \times 20$ mm = 25 mm.

Tube bundle diameter:

$$D_b = 20\left(\frac{992}{0.158}\right)^{1/2.263} = 954 \text{ mm} \tag{19.3b}$$

Number of tubes in center row $N_r = D_b/P_t = 954/25 = 38$

Shell-side coefficient

Estimate tube wall temperature, T_w; assume condensing coefficient of 1500 W/m^2°C:
Mean temperature:

$$\text{Shell}-\text{side} = \frac{60+45}{2} = 52.5^\circ\text{C}$$

$$\text{Tube}-\text{side} = \frac{40+30}{2} = 35^\circ\text{C}$$

$$(52.5 - T_w)1500 = (52.5 - 35)900$$

$$T_w = 42.0^\circ\text{C}$$

$$\text{Mean temperature condensate} = \frac{52.5+42.0}{2} = 47^\circ\text{C}$$

Physical properties at 47 °C:

$$\mu_L = 0.16 \text{ mNs/m}^2$$

$$\rho_L = 551 \text{ kg/m}^3$$

$$k_L = 0.13 \text{ W/m}^\circ\text{C}$$

Vapor density at mean vapor temperature:

$$\rho_v = \frac{52}{22.4} \times \frac{273}{(273+52.5)} \times \frac{10}{1} = 19.5 \text{ kg/m}^3$$

$$\Gamma_h = \frac{W_c}{LN_t} = \frac{45,000}{3600} \times \frac{1}{4.88 \times 992} = 2.6 \times 10^{-3} \text{ kg/s m}$$

$$N_r = \frac{2}{3} \times 38 = 25 \tag{19.29}$$

$$h_c = 0.95 \times 0.13\left[\frac{551(551-19.5)9.81}{0.16 \times 10^{-3} \times 2.6 \times 10^{-3}}\right]^{1/3} \times 25^{-1/6}$$

$$= 1375 \text{ W/m}^{2\circ}\text{C}$$

Close enough to assumed value of 1500 W/m^2°C, so no correction to T_w needed.

Tube-side coefficient

$$\text{Tube cross}-\text{sectional area} = \frac{\pi}{4}\left(16.8 \times 10^{-3}\right)^2 \times \frac{992}{4} = 0.055 \text{ m}^2$$

$$\text{Density of water, at } 35^\circ\text{C} = 993 \text{ kg/m}^3$$

$$\text{Tube velocity} = \frac{104.5}{993} \times \frac{1}{0.055} = 1.91 \text{ m/s} \tag{19.17}$$

$$h_i = \frac{4200(1.35 + 0.02 \times 35)1.91^{0.8}}{16.8^{0.2}}$$

$$= 8218 \text{ W/m}^{2\circ}\text{C}$$

Fouling factors: As neither fluid is heavily fouling, use 6000 W/m^2°C for each side.

$$k_w = 50 \text{ W/m}^\circ\text{C}$$

Overall coefficient

$$\frac{1}{U} = \frac{1}{1375} + \frac{1}{6000} + \frac{20 \times 10^{-3} \ln\left(\frac{20}{16.8}\right)}{2 \times 50} + \frac{20}{16.8} \times \frac{1}{6000} + \frac{20}{16.8} \times \frac{1}{8218} \tag{19.2}$$

$$U = \underline{\underline{786 \text{ W/m}^{2^\circ}\text{C}}}$$

Significantly lower than the assumed value of 900 W/m^2°C.
Repeat calculation using new trial value of 750 W/m^2°C:

$$\text{Area} = \frac{4368 \times 10^3}{750 \times 16} = 364 \text{ m}^2$$

$$\text{Number of tubes} = \frac{364}{0.305} = 1194 \tag{19.3b}$$

$$D_b = 20\left(\frac{1194}{0.158}\right)^{1/2.263} = 1035 \text{ mm}$$

$$\text{Number of tubes in center row} = \frac{1035}{25} = 41$$

$$\Gamma_h = \frac{45,000}{3600} \times \frac{1}{4.88 \times 1194} = 2.15 \times 10^{-3} \text{ kg/m s}$$

$$N_r = \frac{2}{3} \times 41 = 27$$

$$h_c = 0.95 \times 0.13\left[\frac{551(551 - 19.5)9.81}{0.16 \times 10^{-3} \times 2.15 \times 10^{-3}}\right]^{1/3} \times 27^{-1/6}$$

$$= 1447 \text{ W/m}^{2^\circ}\text{C} \tag{19.29}$$

$$\text{New tube velocity} = 1.91 \times \frac{992}{1194} = 1.59 \text{ m/s}$$

$$h_i = 4200(1.35 + 0.02 \times 35)\frac{1.59^{0.8}}{16.8^{0.2}} = 7097 \text{ W/m}^{2^\circ}\text{C} \tag{19.17}$$

$$\frac{1}{U} = \frac{1}{1447} + \frac{1}{6000} + \frac{20 \times 10^{-3} \ln\left(\frac{20}{16.8}\right)}{2 \times 50} + \frac{20}{16.8} \times \frac{1}{6000} + \frac{20}{16.8} \times \frac{1}{7097} \tag{19.2}$$

$$U = \underline{\underline{773 \text{ W/m}^{2^\circ}\text{C}}}$$

Close enough to estimate, firm up design.

Shell-side pressure drop

Use pull-through floating head, no need for close clearance.

Select baffle spacing = shell diameter, 45% cut.
From Fig. 19.10, clearance = 95 mm.
Shell i.d. = 1035 + 95 = 1130 mm
Use Kern's method to make an approximate estimate.

$$\text{Cross-flow area } A_s = \frac{(25 - 20)}{25} 1130 \times 1130 \times 10^{-6} \tag{19.21}$$

$$= 0.255 \text{ m}^2$$

Mass flow rate based on inlet conditions:

$$G_s = \frac{45,000}{3600} \times \frac{1}{0.255} = 49.02 \text{ kg/s m}^2$$

$$\text{Equivalent diameter, } d_e = \frac{1.27}{20}\left(25^2 - 0.785 \times 20^2\right) \tag{19.22}$$

$$= 19.8 \text{ mm}$$

$$\text{Vapor viscosity} = 0.008 \text{ mNs/m}^2$$

$$\text{Re} = \frac{49.02 \times 19.8 \times 10^{-3}}{0.008 \times 10^{-3}} = 121,325$$

From Fig. 19.30, $j_f = 2.2 \times 10^{-2}$:

$$u_s = \frac{G_s}{\rho_v} = \frac{49.02}{19.5} = 2.51 \text{ m/s}$$

Take pressure drop as 50% of that calculated using the inlet flow; neglect viscosity correction.

$$\Delta P_s = \frac{1}{2}\left[8 \times 2.2 \times 10^{-2}\left(\frac{1130}{19.8}\right)\left(\frac{4.88}{1.130}\right)\frac{19.5(2.51)^2}{2}\right] \tag{19.26}$$

$$= 1322 \text{ N/m}^2$$

$$= \underline{\underline{1.3 \text{ kPa}}}$$

Negligible; more sophisticated method of calculation not justified.

Tube-side pressure drop

Viscosity of water = 0.6 mN s/m^2:

$$\text{Re} = \frac{u_t \rho d_i}{\mu} = \frac{1.59 \times 993 \times 16.8 \times 10^{-3}}{0.6 \times 10^{-3}} = 44,208$$

From Fig. 19.24, $j_f = 3.5 \times 10^{-3}$.

Neglect the viscosity correction.

$$\Delta P_t = 4\left[8 \times 3.5 \times 10^{-3}\left(\frac{4.88}{16.8 \times 10^{-3}}\right) + 2.5\right]\frac{993 \times 1.59^2}{2} \tag{19.20}$$

$$= 53,388 \text{ N/m}^2$$

$$= \underline{\underline{53 \text{ kPa}}} \ (7.7 \text{ psi}).$$

This pressure drop is acceptable.

19.11 Reboilers and vaporizers

The design methods given in this section can be used for reboilers and vaporizers. Reboilers are used with distillation columns to vaporize a fraction of the bottom product, whereas in a vaporizer essentially all the feed is vaporized.

Three principal types of reboiler are used:

1. Forced circulation (Fig. 19.46): The fluid is pumped through the exchanger and the vapor formed is separated in the base of the column. When used as a vaporizer, a disengagement vessel must be provided.
2. Thermosiphon, natural circulation (Fig. 19.47): Vertical exchangers with vaporization in the tubes or horizontal exchangers with vaporization in the shell. The liquid circulation through the exchanger is maintained by the

difference in density between the two-phase mixture of vapor and liquid in the exchanger and the single-phase liquid in the base of the column. As with the forced-circulation type, a disengagement vessel will be needed if this type is used as a vaporizer.

3. Kettle type (Fig. 19.48): Boiling takes place on tubes immersed in a pool of liquid; there is no circulation of liquid through the exchanger. This type is also, more correctly, called a submerged bundle reboiler. In some applications it is possible to accommodate the bundle in the base of the column (Fig. 19.49), saving the cost of the exchanger shell. This arrangement is commonly known as a "stab-in" reboiler.

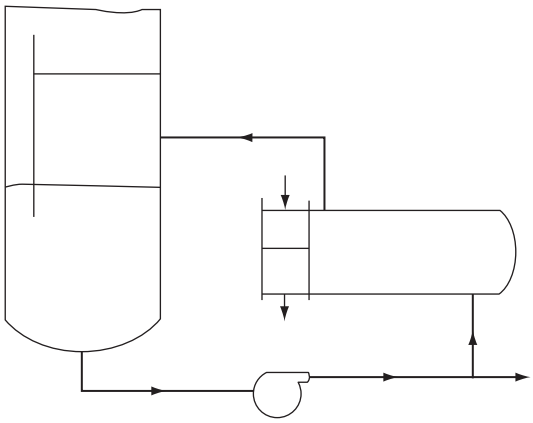


FIG. 19.46 Forced-circulation reboiler.

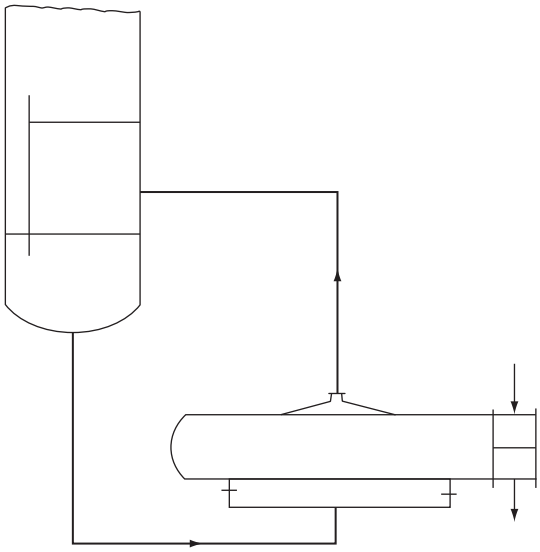


FIG. 19.47 Horizontal thermosiphon reboiler.

Choice of type

The choice of the best type of reboiler or vaporizer for a given duty will depend on the following factors:

1. The nature of the process fluid, particularly its viscosity and propensity to fouling
2. The operating pressure: vacuum or pressure
3. The equipment layout, particularly the headroom available

Forced-circulation reboilers are especially suitable for handling viscous and heavily fouling process fluids; see Chantry and Church (1958). The circulation rate is predictable, and high velocities can be used. They are also suitable for low vacuum operations and for low rates of vaporization. The major disadvantage of this type is that a pump is required and the pumping cost will be high. There is also the danger that leakage of hot fluid could occur at the pump seal; canned-rotor-type pumps can be specified to avoid the possibility of leakage.

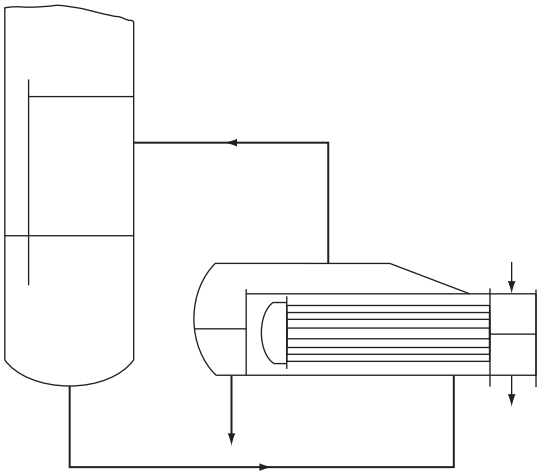


FIG. 19.48 Kettle reboiler.

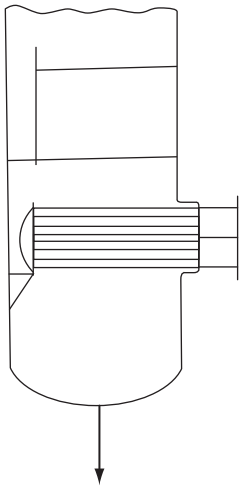


FIG. 19.49 Internal reboiler.

Thermosiphon reboilers are the most economical type for most applications, but are not suitable for high-viscosity fluids or high-vacuum operation. They would not normally be specified for pressures below 0.3 bar. A disadvantage of this type is that the column base must be elevated to provide the hydrostatic head required for the thermosiphon effect. This increases the cost of the column-supporting structure. Horizontal reboilers need less headroom than vertical but have more complex pipework. Horizontal exchangers are easier to maintain than vertical, as the tube bundle is easier to withdraw.

Kettle reboilers have lower heat transfer coefficients than the other types, as there is no liquid circulation. They are not suitable for fouling materials and have a high residence time. They will generally be more expensive than an equivalent thermosiphon type, as a larger shell is needed, but if the duty is such that the bundle can be installed in the column base, the cost will be competitive with the other types. They are often used as vaporizers, as a separate vapor–liquid disengagement vessel is not needed. They are suitable for vacuum operation and for high rates of vaporization, up to 80% of the feed. Some designs allow a liquid blowdown stream to be withdrawn to prevent accumulation of solids or nonvolatile components.

19.11.1 Boiling heat transfer fundamentals

The complex phenomena involved in heat transfer to a boiling liquid are discussed in Chhabra and Shankar (2017). A more detailed account is given by Collier and Thome (1994), Tong and Tang (1997), and Hsu and Graham (1976).

Only a brief discussion of the subject will be given in this section, sufficient for the understanding of the design methods given for reboilers and vaporizers.

The mechanism of heat transfer from a submerged surface to a pool of liquid depends on the temperature difference between the heated surface and the liquid (Fig. 19.50). At low temperature differences, when the liquid is below its boiling point, heat is transferred by natural convection. As the surface temperature is raised, incipient boiling occurs, with vapor bubbles forming and breaking loose from the surface. The agitation caused by the rising bubbles and other effects caused by bubble generation at the surface result in a large increase in the rate of heat transfer. This phenomenon is known as nucleate boiling. As the temperature is raised further, the rate of heat transfer increases until the heat flux reaches a critical value. At this point, the rate of vapor generation is such that dry patches occur spontaneously over the surface and the rate of heat transfer falls off rapidly. At higher temperature differences, the vapor rate is such that the whole surface is blanketed with vapor and the mechanism of heat transfer is by conduction through the vapor film. Conduction is augmented at very high temperature differences by radiation.

The maximum heat flux achievable with nucleate boiling is known as the critical heat flux. In a system where the surface temperature is not self-limiting, such as a nuclear reactor fuel element or a boiling tube that is heated in a fired heater, operation above the critical flux will result in a rapid increase in the surface temperature, and in the extreme situation the surface will melt. This phenomenon is known as "burn-out." The heating media used for process plants are normally self-limiting; for example, with a steam-heated reboiler, the surface temperature can never exceed the saturation temperature of the condensing steam. Care must be taken in the design of electrically heated vaporizers and directly fired vaporizers to ensure that the critical flux can never be exceeded. If the critical flux is exceeded in a directly fired vaporizer, then the tube wall temperature can approach the temperatures of the radiant zone (the bridge-wall temperature or even the flame temperature). At these temperatures damage to the tubes will occur.

The critical flux is reached at surprisingly low temperature differences: around 20 °C to 30 °C for water and 20 °C to 50 °C for light organics.

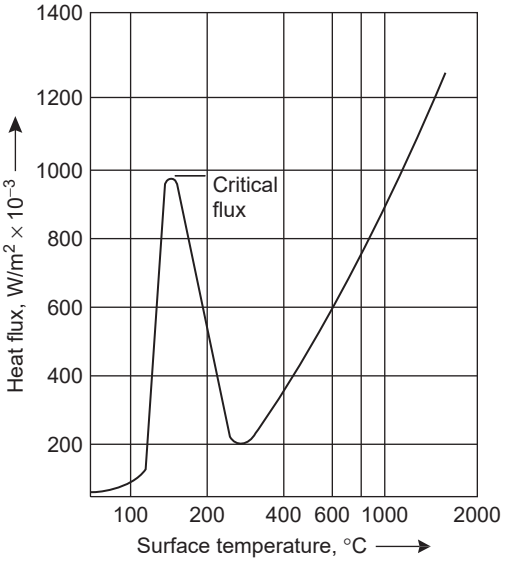


FIG. 19.50 Typical pool boiling curve (water at 1 bar).

Estimation of boiling heat transfer coefficients

In the design of vaporizers and reboilers, the designer will be concerned with two types of boiling: pool boiling and convective boiling. Pool boiling is the name given to nucleate boiling in a pool of liquid, such as in a kettle-type reboiler or a jacketed vessel. Convective boiling occurs where the vaporizing fluid is flowing over the heated surface and heat transfer takes place both by forced convection and nucleate boiling, as in forced circulation or thermosiphon reboilers.

Boiling is a complex phenomenon, and boiling heat transfer coefficients are difficult to predict with any certainty. Whenever possible, experimental values obtained for the system being considered should be used or values for a closely related system.

19.11.2 Pool boiling

In the nucleate boiling region the heat transfer coefficient is dependent on the nature and condition of the heat transfer surface, and it is not possible to present a universal correlation that will give accurate predictions for all systems. Palen and Taborek (1962) have reviewed the published correlations and compared their suitability for use in reboiler design.

The correlation given by Forster and Zuber (1955) can be used to estimate pool boiling coefficients in the absence of experimental data. Their equation can be written in the form:

$$h_{nb} = 0.00122\left[\frac{k_L^{0.79} C_{pL}^{0.45} \rho_L^{0.49}}{\sigma^{0.5} \mu_L^{0.29} \lambda^{0.24} \rho_v^{0.24}}\right](T_w - T_s)^{0.24}(p_w - p_s)^{0.75} \tag{19.41}$$

where h_{nb} = nucleate, pool, boiling coefficient, W/m^2°C
k_L = liquid thermal conductivity, W/m°C
C_{pL} = liquid heat capacity, J/kg°C
ρ_L = liquid density, kg/m^3
μ_L = liquid viscosity, Ns/m^2
λ = latent heat, J/kg
ρ_v = vapor density, kg/m^3
T_w = wall, surface temperature, °C
T_s = saturation temperature of boiling liquid °C
p_w = saturation pressure corresponding to the wall temperature, T_w, N/m^2
p_s = saturation pressure corresponding to T_s, N/m^2
σ = surface tension, N/m

The reduced-pressure correlation given by Mostinski (1963) is simple to use and gives values that are as reliable as those given by more complex equations.

$$h_{nb} = 0.104(P_c)^{0.69}(q)^{0.7}\left[1.8\left(\frac{P}{P_c}\right)^{0.17} + 4\left(\frac{P}{P_c}\right)^{1.2} + 10\left(\frac{P}{P_c}\right)^{10}\right] \tag{19.42}$$

where P = operating pressure, bar
P_c = liquid critical pressure, bar
q = heat flux, W/m^2
Note: $q = h_{nb}(T_w - T_s)$.

Mostinski's equation is convenient to use when data on the fluid physical properties are not available.

Equations 19.41 and 19.42 are for boiling single-component fluids; for mixtures, the coefficient will generally be lower than is predicted by these equations. The equations can be used for close boiling range mixtures, say less than 5 °C, and for wider boiling ranges with a suitable factor of safety (see Section 19.11.6).

Critical heat flux

It is important to check that the design and operating heat fluxes are well below the critical flux. Several correlations are available for predicting the critical flux. That given by Zuber et al. (1961) has been found to give satisfactory predictions for use in reboiler and vaporizer design. In SI units, Zuber's equation can be written as:

$$q_c = 0.131\lambda\left[\sigma g(\rho_L - \rho_v)\rho_v^2\right]^{1/4} \tag{19.43}$$

where q_c = maximum, critical, heat flux, W/m^2
g = gravitational acceleration, 9.81 m/s^2

Mostinski also gives a reduced-pressure equation for predicting the maximum critical heat flux:

$$q_c = 3.67 \times 10^4 P_c\left(\frac{P}{P_c}\right)^{0.35}\left[1 - \left(\frac{P}{P_c}\right)\right]^{0.9} \tag{19.44}$$

Film boiling

The equation given by Bromley (1950) can be used to estimate the heat transfer coefficient for film boiling on tubes. Heat transfer in the film-boiling region will be controlled by conduction through the film of vapor, and Bromley's equation is similar to the Nusselt equation for condensation, where conduction is occurring through the film of condensate.

$$h_{fb} = 0.62\left[\frac{k_v^3(\rho_L - \rho_v)\rho_v g\lambda}{\mu_v d_o(T_w - T_s)}\right]^{1/4} \tag{19.45}$$

where h_{fb} is the film boiling heat transfer coefficient, the suffix v refers to the vapor phase, and d_o is in meters. It must be emphasized that process reboilers and vaporizers will always be designed to operate in the nucleate boiling region. The heating medium would be selected, and its temperature controlled, to ensure that in operation the temperature difference is well below that at which the critical flux is reached. For instance, if direct heating with steam would give too high a temperature difference, the steam would be used to heat water and hot water used as the heating medium. Above temperatures where steam can be used, hot oil circuits are often used for reboilers so as to avoid direct firing of the reboiler.

Example 19.8

Estimate the heat transfer coefficient for the pool boiling of water at 2.1 bar from a surface at 125 °C. Check that the critical flux is not exceeded.

Solution

Physical properties, from steam tables:

Saturation temperature, $T_s = 121.8°C$

$$\rho_L = 941.6\ \text{kg/m}^3,\quad \rho_v = 1.18\ \text{kg/m}^3$$

$$C_{pL} = 4.25 \times 10^3\ \text{J/kg°C}$$

$$k_L = 687 \times 10^{-3}\ \text{Wm°C}$$

$$\mu_L = 230 \times 10^{-6}\ \text{Ns/m}^2$$

$$\lambda = 2198 \times 10^3\ \text{J/kg}$$

$$\sigma = 55 \times 10^{-3}\ \text{N/m}$$

$$p_w \text{ at } 125°C = 2.321 \times 10^5\ \text{N/m}^2$$

$$p_s = 2.1 \times 10^5\ \text{N/m}^2$$

Use the Foster–Zuber correlation (Equation 19.41):

$$h_{nb} = 1.22 \times 10^{-3}\left[\frac{(687\times 10^{-3})^{0.79}(4.25\times 10^3)^{0.45}(941.6)^{0.49}}{(55\times 10^{-3})^{0.5}(230\times 10^{-6})^{0.29}(2198\times 10^3)^{0.24}(1.18)^{0.24}}\right](125-121.8)^{0.24}(2.321\times 10^5 - 2.1\times 10^5)^{0.75}$$

$$= 3738\ \text{W/m}^{2\circ}\text{C}$$

Use the Zuber correlation (Equation 19.43):

$$q_c = 1.131 \times 2198 \times 10^3\left[55 \times 10^{-3} \times 9.81(941.6 - 1.18)1.18^2\right]^{1/4}$$

$$= \underline{\underline{1.48 \times 10^6\ \text{W/m}^2}}$$

$$\text{Actual flux} = (125 - 121.8)\,3738 = \underline{\underline{11,962\ \text{W/m}^2}}$$

well below critical flux.

19.11.3 Convective boiling

The mechanism of heat transfer in convective boiling, where the boiling fluid is flowing through a tube or over a tube bundle, differs from that in pool boiling. It will depend on the state of the fluid at any point. Consider the situation of a liquid boiling inside a vertical tube (Fig. 19.51). The following conditions occur as the fluid flows up the tube:

1. Single-phase flow region: At the inlet, the liquid is below its boiling point (subcooled) and heat is transferred by forced convection. The equations for forced convection can be used to estimate the heat transfer coefficient in this region.
2. Subcooled boiling: In this region the liquid next to the wall has reached the boiling point, but not the bulk of the liquid. Local boiling takes place at the wall, which increases the rate of heat transfer over that given by forced convection alone.
3. Saturated boiling region: In this region bulk boiling of the liquid is occurring in a manner similar to nucleate pool boiling. The volume of vapor is increasing, and various flow patterns can form. In a long tube, the flow pattern will eventually become annular, where the liquid phase is spread over the tube wall and the vapor flows up the central core.
4. Dry wall region: Ultimately, if a large fraction of the feed is vaporized, the wall dries out and any remaining liquid is present as a mist. Heat transfer in this region is by convection and radiation to the vapor. This condition is unlikely to occur in commercial reboilers and vaporizers.

Saturated, bulk, boiling is the principal mechanism of interest in the design of reboilers and vaporizers.

A comprehensive review of the methods available for predicting convective boiling coefficients is given by Webb and Gupte (1992). The methods proposed by Chen (1966) and Shah (1976) are convenient to use in manual calculations and are accurate enough for preliminary design work. Chen's method is outlined next and illustrated in Example 19.9.

Chen's method

In forced-convective boiling, the effective heat transfer coefficient h_{cb} can be considered to be made up of convective and nucleate boiling components: h'_{fc} and h'_{nb}.

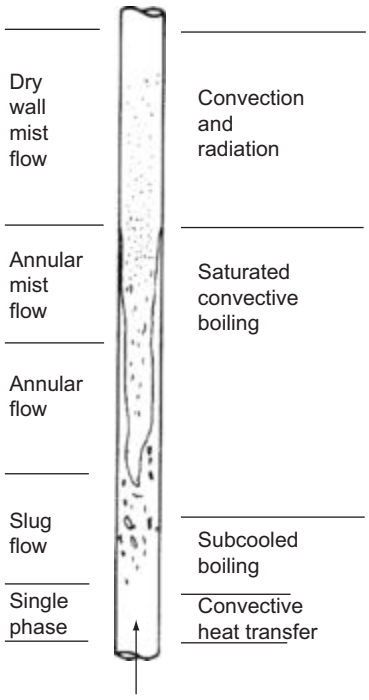


FIG. 19.51 Convective boiling in a vertical tube.

$$h_{cb} = h'_{fc} + h'_{nb} \tag{19.46}$$

The convective boiling coefficient h'_{fc} can be estimated using the equations for single-phase forced-convection heat transfer modified by a factor f_c to account for the effects of two-phase flow:

$$h'_{fc} = h_{fc} \times f_c \tag{19.47}$$

The forced-convection coefficient h_{fc} is calculated assuming that the liquid phase is flowing in the conduit alone.

The two-phase correction factor f_c is obtained from Fig. 19.52 in which the term $1/X_{tt}$ is the Lockhart–Martinelli two-phase flow parameter with turbulent flow in both phases (see Chhabra & Shankar 2017). This parameter is given by:

$$\frac{1}{X_{tt}} = \left[\frac{x}{1-x}\right]^{0.9} \left[\frac{\rho_L}{\rho_v}\right]^{0.5} \left[\frac{\mu_v}{\mu_L}\right]^{0.1} \tag{19.48}$$

where x is the vapor quality, the mass fraction of vapor.

The nucleate boiling coefficient can be calculated using correlations for nucleate pool boiling modified by a factor f_s to account for the fact that nucleate boiling is more difficult in a flowing liquid.

$$h'_{nb} = h_{nb} \times f_s \tag{19.49}$$

The suppression factor f_s is obtained from Fig. 19.53. It is a function of the liquid Reynolds number Re_L and the forced-convection correction factor f_c.

Re_L is evaluated assuming that only the liquid phase is flowing in the conduit and will be given by:

$$\mathrm{Re}_L = \frac{(1 - x)\, G\, d_e}{\mu_L} \tag{19.50}$$

where G is the total mass flow rate per unit flow area.

Chen's method was developed from experimental data on forced convective boiling in vertical tubes. It can be applied, with caution, to forced convective boiling in horizontal tubes and annular conduits (concentric pipes).

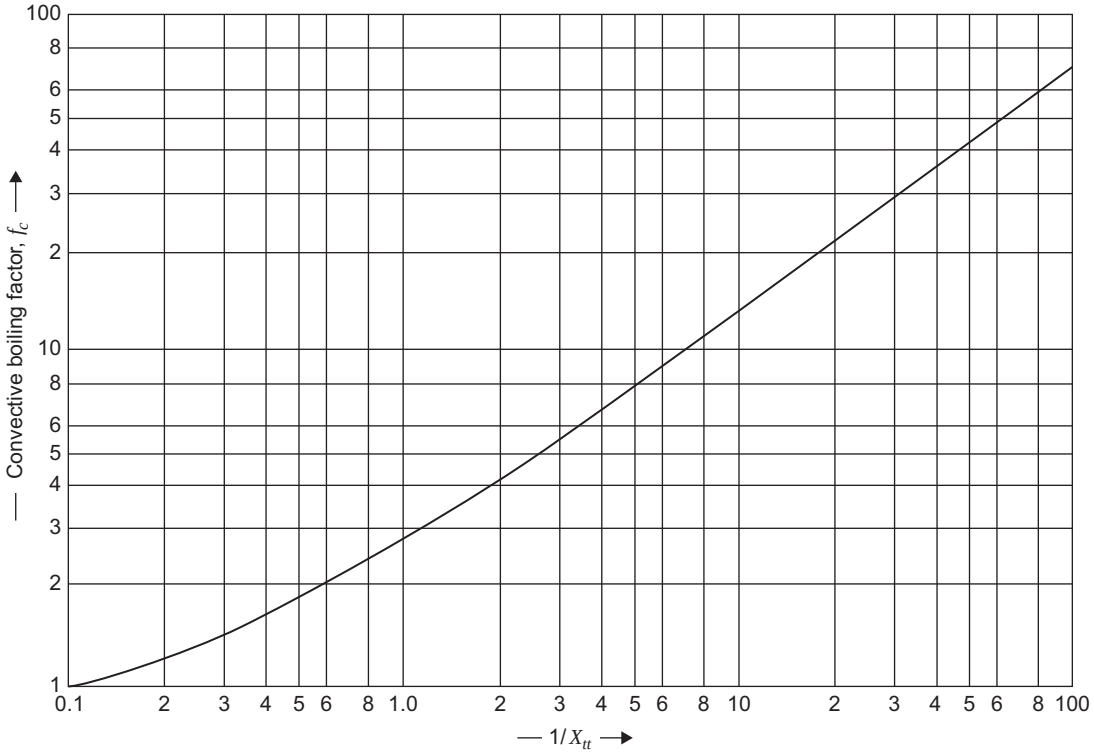


FIG. 19.52 Convective boiling enhancement factor.

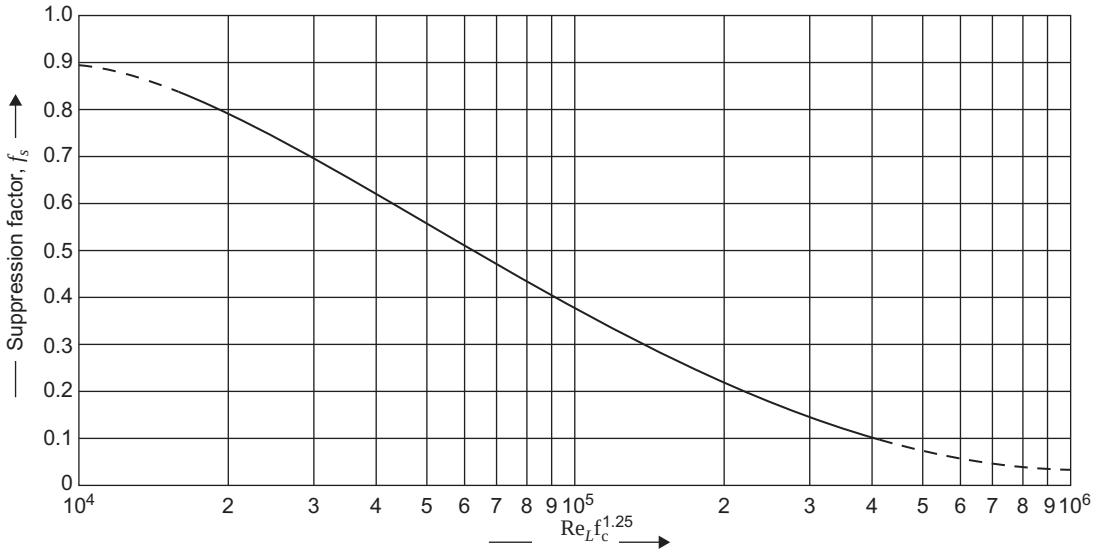


FIG. 19.53 Nucleate boiling suppression factor.

Butterworth (1977) suggests that in the absence of more reliable methods, it may be used to estimate the heat transfer coefficient for forced convective boiling in cross flow over tube bundles, using a suitable cross-flow correlation to predict the forced-convection coefficient. Shah's method was based on data for flow in horizontal and vertical tubes and annuli.

A major problem that will be encountered when applying convective boiling correlations to the design of reboilers and vaporizers is that because the vapor quality changes progressively throughout the exchanger, a step-by-step procedure will be needed. The exchanger must be divided into sections and the coefficient and heat transfer area estimated sequentially for each section.

Example 19.9

A fluid whose properties are essentially those of o-dichlorobenzene is vaporized in the tubes of a forced convection reboiler. Estimate the local heat transfer coefficient at a point where 5% of the liquid has been vaporized. The liquid velocity at the tube inlet is 2 m/s, and the operating pressure is 0.3 bar. The tube inside diameter is 16 mm, and the local wall temperature is estimated to be 120 °C.

Solution

Physical properties:

boiling point 136 °C

$\rho_L = 1170$ kg/m^3

$\mu_L = 0.45$ mNs/m^2

$\mu_v = 0.01$ mNs/m^2

$\rho_v = 1.31$ kg/m^3

$k_L = 0.11$ W/m°C

$C_{pL} = 1.25$ kJ/kg°C

$P_c = 41$ bar

The forced-convective boiling coefficient will be estimated using Chen's method.

With 5% vapor, liquid velocity (for liquid flow in tube alone):

$$= 2 \times 0.95 = 1.90 \text{ m/s}$$

$$\text{Re}_L = \frac{1170 \times 1.90 \times 16 \times 10^{-3}}{0.45 \times 10^{-3}} = 79,040$$

From Fig. 19.23, $j_h = 3.3 \times 10^{-3}$:

$$\text{Pr} = \frac{1.25 \times 10^3 \times 0.45 \times 10^{-3}}{0.11} = 5.1$$

Neglect viscosity correction term:

$$h_{fc} = \frac{0.11}{16 \times 10^{-3}} \times 3.3 \times 10^{-3}(79,040)(5.1)^{0.33} \tag{19.15}$$

$$= 3070 \text{ W/m}^{2\circ}\text{C}$$

$$\frac{1}{X_{tt}} = \left[\frac{0.05}{1-0.05}\right]^{0.9}\left[\frac{1170}{1.31}\right]^{0.5}\left[\frac{0.01 \times 10^{-3}}{0.45 \times 10^{-3}}\right]^{0.1} \tag{19.48}$$

$$= 1.44$$

From Fig. 19.52, $f_c = 3.2$:

$$h'_{fc} = 3.2 \times 3070 = 9824 \text{ W/m}^{2\circ}\text{C}$$

Using Mostinski's correlation to estimate the nucleate boiling coefficient:

$$h_{nb} = 0.104 \times 41^{0.69}[h_{nb}(136 - 120)]^{0.7}\left[1.8\left(\frac{0.3}{41}\right)^{0.17} + 4\left(\frac{0.3}{41}\right)^{1.2} + 10\left(\frac{0.3}{41}\right)^{10}\right]$$

$$h_{nb} = 7.43\, h_{nb}^{0.7} \tag{19.42}$$

$$h_{nb} = 800 \text{ W/m}^{2\circ}\text{C}$$

$$\text{Re}_L f_c^{1.25} = 79,040 \times 3.2^{1.25} = 338,286$$

From Fig. 19.53, $f_s = 0.13$:

$$h'_{nb} = 0.13 \times 800 = 104 \text{ W/m}^{2\circ}\text{C}$$

$$h_{cb} = 9824 + 104 = \underline{\underline{9928 \text{ W/m}^{2\circ}\text{C}}}$$

19.11.4 Design of forced-circulation reboilers

The normal practice in the design of forced-convection reboilers is to calculate the heat transfer coefficient, assuming that the heat is transferred by forced convection only. This will give conservative (safe) values, as any boiling that occurs will invariably increase the rate of heat transfer. In many designs, the pressure is controlled to prevent any appreciable vaporization in the exchanger. A throttle value is installed in the exchanger outlet line, and the liquid flashes as the pressure is let down into the vapor–liquid separation vessel.

If a significant amount of vaporization does occur, the heat transfer coefficient can be evaluated using correlations for convective boiling, such as Chen's method.

Conventional shell and tube exchanger designs are used with one shell pass and two tube passes when the process fluid is on the shell side and with one shell and one tube pass when it is in the tubes. High tube velocities

are used to reduce fouling: 3 to 9 m/s. Because the circulation rate is set by the designer, forced-circulation reboilers can be designed with more certainty than natural-circulation units.

The critical flux in forced-convection boiling is difficult to predict. Kern (1950) recommends that for commercial reboiler designs the heat flux should not exceed 63,000 W/m^2 (20,000 Btu/ft^2h) for organics and 95,000 W/m^2 (30,000 Btu/ft^2h) for water and dilute aqueous solutions. These values are now generally considered to be too pessimistic.

19.11.5 Design of thermosiphon reboilers

The design of thermosiphon reboilers is complicated by the fact that, unlike a forced-convection reboiler, the fluid circulation rate cannot be determined explicitly. The circulation rate, heat transfer rate, and pressure drop are all interrelated, and iterative design procedures must be used. The fluid will circulate at a rate at which the pressure losses in the system are just balanced by the available hydrostatic head. The exchanger, column base, and piping act like two legs of a U-tube (Fig. 19.54). The driving force for circulation around the system is the difference in density of the liquid in the "cold" leg (the column base and inlet piping) and the two-phase fluid in the "hot" leg (the exchanger tubes and outlet piping).

To calculate the circulation rate, it is necessary to make a pressure balance around the system. A typical design procedure will include the following steps:

1. Calculate the vaporization rate required from the specified duty.
2. Estimate the exchanger area from an assumed value for the overall heat transfer coefficient. Decide the exchanger layout and piping dimensions.
3. Assume a value for the circulation rate through the exchanger.
4. Calculate the pressure drop in the inlet piping (single phase).
5. Divide the exchanger tube into sections and calculate the pressure drop section by section up the tube. Use suitable methods for the sections in which the flow is two-phase. Include the pressure loss due to the fluid acceleration as the vapor rate increases. For a horizontal reboiler, calculate the pressure drop in the shell, using a method suitable for two-phase flow.
6. Calculate the pressure drop in the outlet piping (two-phase).
7. Compare the calculated pressure drop with the available differential head, which will depend on the vapor voidage, and hence the assumed circulation rate. If a satisfactory balance has been achieved, proceed. If not, return to step 3 and repeat the calculations with a new assumed circulation rate.
8. Calculate the heat transfer coefficient and heat transfer rate section by section up the tubes. Use a suitable method for the sections in which the boiling is occurring, such as Chen's method.

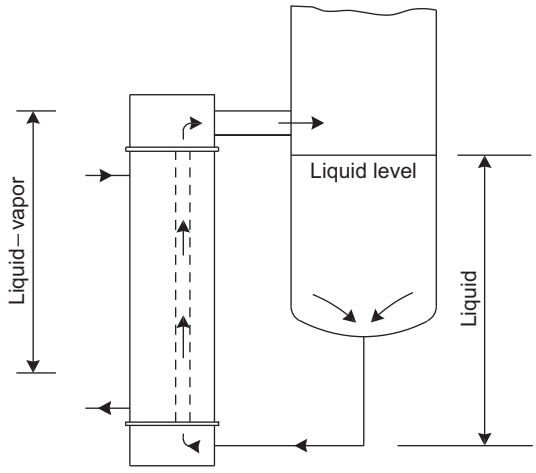


FIG. 19.54 Vertical thermosiphon reboiler, liquid and vapor flows.

9. Calculate the rate of vaporization from the total heat transfer rate, and compare with the value assumed in step 1. If the values are sufficiently close, proceed. If not, return to step 2 and repeat the calculations for a new design.
10. Check that the critical heat flux is not exceeded at any point up the tubes.
11. Repeat the complete procedure as necessary to optimize the design.

It can be seen that to design a thermosiphon reboiler using hand calculations would be tedious and time-consuming. The iterative nature of the procedure lends itself to solution by computers. Sarma et al. (1973) discuss the development of a computer program for vertical thermosiphon reboiler design and give algorithms and design equations.

Extensive work on the performance and design of thermosiphon reboilers has been carried out by HTFS and HTRI, and proprietary design programs are available from these organizations. The HTFS methods are available in Aspen Technology's Aspen Engineering Suite and in Honeywell's UniSim Design Suite; see Table 4.1.

In the absence of access to a computer program, the rigorous design methods given by Fair (1960, 1963) or Hughmark (1961, 1964, 1969) can be used for thermosiphon vertical reboilers. Collins (1976) and Fair and Klip (1983) give methods for the design of horizontal, shell-side thermosiphon reboilers. The design and performance of this type of reboiler is also reviewed in a paper by Yilmaz (1987).

Approximate methods can be used for preliminary designs. Fair (1960) gives a method in which the heat transfer and pressure drop in the tubes are based on the average of the inlet and outlet conditions. This simplifies step 5 in the design procedure, but trial-and-error calculations are still needed to determine the circulation rate. Frank and Prickett (1973) programmed Fair's rigorous design method for computer solution and used it, together with operating data on commercial exchangers, to derive a general correlation of heat transfer rate with reduced temperature for vertical thermosiphon reboilers. Their correlation, converted to SI units, is shown in Fig. 19.55. The basis and limitations of the correlation are as follows:

1. Conventional designs: tube lengths 2.5 to 3.7 m (8 to 12 ft) (standard length 2.44 m), preferred diameter 25 mm (1 in.)
2. Liquid in the sump level with the top tubesheet
3. Process-side fouling coefficient 6000 W/m$^{2\circ}$C
4. Heating medium steam, coefficient including fouling, 6000 W/m$^{2\circ}$C
5. Simple inlet and outlet piping
6. For reduced temperatures greater than 0.8, use the limiting curve (that for aqueous solutions)
7. Minimum operating pressure 0.3 bar
8. Inlet fluid should not be appreciably subcooled
9. Extrapolation is not recommended

For heating media other than steam and process-side fouling coefficients different from 6000 W/m$^{2\circ}$C, the design heat flux taken from Fig. 19.55 may be adjusted as follows:

$$U' = \frac{q'}{\Delta T'} \tag{19.51}$$

and

$$\frac{1}{U_c} = \frac{1}{U'} - \frac{1}{6000} + \frac{1}{h_s} - \frac{1}{6000} + \frac{1}{h_{id}}$$

Where q' = flux read from Fig. 19.55 at $\Delta T'$
h_s = new shell-side coefficient, W/m$^{2\circ}$C
h_{id} = fouling coefficient on the process (tube) side W/m$^{2\circ}$C
U_c = corrected overall coefficient

The use of Frank and Prickett's method is illustrated in Example 19.10.

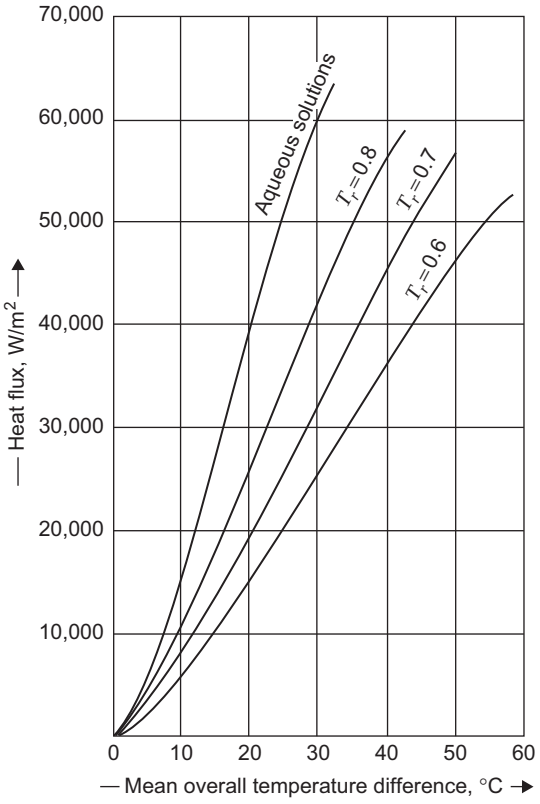


FIG. 19.55 Vertical thermosiphon design correlation.

Limitations on the use of Frank and Prickett's method

A study by van Edmonds (1994) using the HTFS TREB4 program found that Frank and Prickett's method gave acceptable predictions for pure components and binary mixtures with water but that the results were unreliable for other mixtures. Also, van Edmonds's results predicted higher flux values than those obtained by Prickett and Frank.

For preliminary designs for pure components, or near-pure components, Prickett and Frank's method should give a conservative estimate of the operating heat flux. It is not recommended for mixtures other than binary mixtures with water.

Approximate design method for mixtures

For mixtures, the simplified analysis used by Kern (1954) can be used to obtain an approximate estimate of the number of tubes required; see also Aerstin and Street (1978) and Hewitt et al. (1994).

This method uses simple, unsophisticated methods to estimate the two-phase pressure drop through the exchanger and piping and the convective boiling heat transfer coefficient. The calculation procedure is set out next and illustrated in Example 19.11.

Procedure

1. Determine the heat duty.
2. Estimate the heat transfer area using the maximum allowable heat flux. Take as 39,700 W/m^2 for vertical and 47,300 W/m^2 for horizontal reboilers.
3. Choose the tube diameters and length. Calculate the number of tubes required.
4. Estimate the recirculation ratio, not less than 3.
5. Calculate the vapor flow rate leaving the reboiler for the duty and liquid heat of vaporization.
6. Calculate the liquid flow rate leaving the reboiler for the vapor rate and recirculation ratio.
7. Estimate the two-phase pressure drop though the tubes due to friction. Use the homogenous model or another simple method, such as the Lochart–Martenelli equation.
8. Estimate the static head in the tubes.
9. Estimate the available head.
10. Compare the total estimated pressure drop and the available head. If the available head is greater by a sufficient amount to allow for the pressure drop through the inlet and outlet piping, proceed. If the available head is not sufficient, return to step 2 and increase the number of tubes.

11. Calculate the convective heat transfer coefficient using simple methods, such as assuming convection only, or Chen's method; see Section 19.11.3.
12. Calculate the overall heat transfer coefficient.
13. Calculate the required overall coefficient and compare with that estimated. If satisfactory, accept the design; if unsatisfactory, return to step 2 and increase the estimated area.

Maximum heat flux

Thermosiphon reboilers can suffer from flow instabilities if too high a heat flux is used. The liquid and vapor flow in the tubes is not smooth but tends to pulsate, and at high heat fluxes the pulsations can become large enough to cause vapor locking. A good practice is to install a flow restriction in the inlet line, a valve or orifice plate, so that the flow resistance can be adjusted should vapor locking occur in operation.

Kern recommends that the heat flux in thermosiphon reboilers, based on the total heat transfer area, should not exceed 37,900 W/m^2 (12,000 Btu/ft^{2}h). For horizontal thermosiphon reboilers, Collins recommends a maximum flux ranging from 47,300 W/m^2 for 20-mm tubes to 56,800 W/m^2 for 25-mm tubes (15,000 to 18,000 Btu/ft^{2}h). These "rule of thumb" values are now thought to be too conservative; see Shellene et al. (1968) and Furzer (1990). Correlations for determining the maximum heat flux for vertical thermosiphons are given by Lee et al. (1956) and Palen et al. (1974) and for horizontal thermosiphons by Yilmaz (1987).

General design considerations

The tube lengths used for vertical thermosiphon reboilers vary from 1.83 m (6 ft) for vacuum service to 3.66 m (12 ft) for pressure operation. A good size for general applications is 2.44 m (8 ft) by 25 mm internal diameter. Larger tube diameters, up to 50 mm, are used for fouling systems.

The top tubesheet is normally aligned with the liquid level in the base of the column (Fig. 19.54). The outlet pipe should be as short as possible and have a cross-sectional area at least equal to the total cross-sectional area of the tubes.

Example 19.10

Make a preliminary design for a vertical thermosiphon for a column distilling crude aniline. The column will operate at atmospheric pressure, and a vaporization rate of 6000 kg/h is required. Steam is available at 22 bar (300 psig). Take the column bottom pressure as 1.2 bar.

Solution

Physical properties, taken as those of aniline:

Boiling point at 1.2 bar 190 °C
Molecular weight 93.13
T_c 699 K
Latent heat 42,000 kJ/kmol
Steam saturation temperature 217 °C
Mean overall $\Delta T = (217 - 190) = 27$ °C

$$\text{Reduced temperature, } T_r = \frac{(190 + 273)}{699} = 0.66$$

From Fig. 19.55, design heat flux = 25,000 W/m^2

$$\text{Heat load} = \frac{6000}{3600} \times \frac{42,000}{93.13} = 751 \text{ kW}$$

$$\text{Area required} = \frac{751 \times 10^3}{25,000} = 30 \text{ m}^2$$

Use 25 mm i.d., 30 mm o.d., 2.44 m long tubes.

$$\text{Area of one tube} = \pi \times 25 \times 10^{-3} \times 2.44 = 0.192 \text{ m}^2$$

$$\text{Number of tubes} = \frac{30}{0.192} = 157$$

Approximate diameter of bundle, for 1.25 square pitch:

$$D_b = 30\left[\frac{157}{0.215}\right]^{1/2.207} = 595 \text{ mm} \tag{19.3b}$$

A fixed tubesheet will be used for a vertical thermosiphon reboiler. From Fig. 19.10, shell diametrical clearance = 14 mm:

$$\text{Shell inside dia.} = 595 + 14 = 609 \text{ mm}$$

Outlet pipe diameter; take area as equal to total tube cross-sectional area:

$$= 157(25 \times 10^{-3})^2 \frac{\pi}{4} = 0.077 \text{ m}^2$$

$$\text{Pipe diameter} = \sqrt{\frac{0.077 \times 4}{\pi}} = 0.31 \text{ m}$$

Example 19.11

Make a preliminary design for a vertical thermosiphon reboiler for a debutanizer column that has the bottoms composition given here. Take the vapor rate required to be 36 kmol/h.

Bottoms composition: C_3 0.001, iC_4 0.001, nC_4 0.02, iC_5 0.34, nC_5 0.64, kmol.

Operating pressure 8.3 bar. Bubble point of mixture, approximately, 120 °C.

Solution

The concentrations of C_3 and iC_4 are small enough to be neglected.

Take the liquid:vapor ratio as 3:1.

Estimate the liquid and vapor compositions leaving the reboiler:

$$\text{Vapor rate, } V = 36/3600 = 0.1 \text{ kmol/s}$$

$$L/V = 3, \text{ so liquid rate, } L = 3V = 0.3 \text{ kmol/s and feed, } F = L + V = 0.4 \text{ kmol/s}$$

The vapor and liquid compositions leaving the reboiler can be estimated using the same procedure as that for a flash calculation; see Section 17.3.3.

	K_i	$A_i = K_i \times L/V$	$V_i = z_i/(1 + A_i)$	$y_i = V_i/V$	$x_i = (Fz_i\text{-}V_i)/L$
nC_4	2.03	6.09	0.001	0.010	0.023
iC_5	1.06	3.18	0.033	0.324	0.343
nC_5	0.92	2.76	0.068	0.667	0.627
			——	——	——
Totals			0.102	1.001	0.993

Enthalpies of vaporization, kJ/mol (taken from Maxwell 1962):

	x_i	$\Delta H_{vap,i}$	$x_i\ \Delta H_{vap,i}$
nC_4	0.02	16	0.32
iC_5	0.35	17	5.95
nC_5	0.63	19	11.97
			——
Total			18.24

Exchanger duty, feed to reboiler taken as at its boiling point:

$$= \text{vapor flow rate} \quad \text{heat of vaporization}$$

$$= 0.1 \times 10^3 \times 18.24 = \underline{\underline{1824}} \text{ kW}$$

(Note: We could also have estimated this using a nonadiabatic flash model in a process simulation program.)

Take the maximum flux as 37,900 W/m^2; see Section 19.11.5.

$$\text{Heat transfer area required} = 1,824,000/37,900 = 48.1 \text{ m}^2$$

Use 25 mm i.d., 2.5 m long tubes, a popular size for vertical thermosiphon reboilers.

$$\text{Area of one tube} = 25 \times 10^{-3}\pi \times 2.5 = 0.196 \text{ m}^2$$

$$\text{Number of tubes required} = 48.1/0.196 = 246$$

$$\text{Liquid density at base of exchanger} = 520 \text{ kg/m}^3$$

$$\text{Relative molecular mass at tube entry} = 58 \times 0.02 + 72(0.34 + 0.64) = 71.7$$

$$\text{vapor at exit} = 58 \times 0.02 + 72(0.35 + 0.63) = 71.7$$

Two-phase fluid density at tube exit:

$$\text{volume of vapor} = 0.1 \times (22.4/8.3) \times (393/273) = 0.389 \text{ m}^3$$

$$\text{volume of liquid} = (0.3 \times 71.7)/520 = 0.0413 \text{ m}^3$$

$$\text{total volume} = 0.389 + 0.0413 = 0.430 \text{ m}^3$$

$$\text{exit density} = \frac{(0.4 \times 71.7)}{0.430} \times 71.7 = 66.7 \text{ kg/m}^3$$

Friction loss

$$\text{Mass flow rate} = 0.4 \times 71.7 = 28.68 \text{ kg/s}$$

$$\text{Cross} - \text{sectional area of tube} = \frac{\pi(25 \times 10^{-3})^2}{4} = 0.00049 \text{ m}^2$$

$$\text{Total cross} - \text{sectional area of bundle} = 246 \times 0.00049 = 0.121 \text{ m}^2$$

$$\text{Mass flux, G} = \text{mass flow/area} = 28.68/0.121 = 237.0 \text{ kg m}^{-2}\text{s}^{-1}$$

At tube exit, pressure drop per unit length, using the homogeneous model:

$$\text{Homogeneous velocity} = G/\rho_m = 237/66.7 = 3.55 \text{ m/s}$$

$$\text{Viscosity, taken as that of liquid, } = 0.12 \text{ mNsm}^{-2}$$

$$\text{Re} = \frac{\rho_m u d}{\mu} = \frac{66.7 \times 3.55 \times 25 \times 10^{-3}}{0.12 \times 10^{-3}} = 49,330$$

$$\text{Friction factor, from Fig. 19.24} = 3.2 \times 10^{-3}$$

$$\Delta P_f = 8 \times 3.2 \times 10^{-3} \times \frac{1}{25 \times 10^{-3}} \times 66.7 \times \frac{3.55^2}{2} = 430 \text{ N/m}^{-2}\text{per m} \quad (19.19)$$

At tube entry, liquid only, pressure drop per unit length:

$$\text{velocity} = G/\rho_L = 237.0/520 = 0.46 \text{ m/s}$$

$$\text{Re} = \frac{\rho_L u d}{\mu} = \frac{520 \times 0.46 \times 25 \times 10^{-3}}{0.12 \times 10^{-3}} = 49,833$$

Friction factor, from Fig 19.24 $= 3.2 \times 10^{-3}$

$$\Delta P_f = 8 \times 3.2 \times 10^{-3} \times \frac{1}{25 \times 10^{-3}} \times 520 \times \frac{0.46^2}{2} = 56 \text{ N/m}^{-2}\text{per m} \quad (19.19)$$

Taking the pressure drop change as linear along the tube:

$$\text{Mean pressure drop per unit length} = (430+56)/2 = 243\ \text{N/m}^2$$

$$\text{Pressure drop over tube } 243 \times 2.5 = 608\ \text{N/m}^2$$

The viscosity correction factor is neglected in this rough calculation.

Static pressure in tubes

Making the simplifying assumption that the variation in density in the tubes is linear from bottom to top, the static pressure will be given by:

$$\Delta P_s = g\int_0^L \frac{dx}{v_i + x(v_0 - v_i)/L} = \frac{gL}{(v_0 - v_i)} \times \text{Ln}(v_0/v_i)$$

where v_i and v_0 are the inlet and outlet specific volumes.

$$v_i = 1/520 = 0.00192 \text{ and } v_0 = 1/66.7 = 0.0150\ \text{m}^3/\text{kg}$$

$$\Delta P_s = \frac{9.8 \times 2.5}{(0.0150 - 0.00192)} \times \text{Ln}(0.0150/0.00192) = 3850\ \text{N/m}^2$$

Total pressure drop over tubes $= 608 + 3850 = \underline{\underline{4460}}\ \text{N/m}^2$

Available head (driving force)

$$\Delta Ps = \rho_L g L = 520 \times 9.8 \times 2.5 = \underline{\underline{12,740}}\ \text{N/m}^2$$

This is adequate to maintain a circulation ratio of 3:1, including allowances for the pressure drop across the piping.

Heat transfer

The convective boiling coefficient will be calculated using Chen's method; see Section 19.13.3. As the heat flux is known and only a rough estimate of the coefficient is required, use Mostinski's equation to estimate the nucleate boiling coefficient; see Section 19.11.2.

Take the critical pressure as that for n-pentane, 33.7 bar.

$$\begin{aligned} h_{nb} &= 0.104(33.7)^{0.69}(37,900)^{0.7}\left[1.8(8.3/33.7)^{0.17} + 4(8.3/33.7)^{1.2} + 10(8.3/33.7)^{10}\right] \\ &= 1888.6(1.418 + 0.744 + 0.000) = 4083\ \text{Wm}^{-2\circ}\text{C}^{-1} \end{aligned} \tag{19.42}$$

Vapor quality, x = mass vapor/total mass flow $= 0.1/0.4 = 0.25$

Viscosity of vapor $= 0.0084\ \text{mNm}^{-2}\text{s}$

Vapor density at tube exit $= (0.1 \times 71.7)/0.389 = 18.43\ \text{kg/m}^3$

$$1/X_{tt} = [0.25/(1-0.25)]^{0.9}[520/18.43]^{0.5}[0.0084/0.12]^{0.1} = 1.51$$

Specific heat of liquid $= 2.78\ \text{kJkg}^{-1\circ}\text{C}^{-1}$, thermal conductivity of liquid $= 0.12\ \text{W/m}^\circ\text{C}$ (19.46)

$$\text{Pr}_L = \left(2.78 \times 10^3 \times 0.12 \times 10^{-3}\right)/0.12 = 2.78$$

Mass flux, liquid phase only flowing in tubes $= (0.3 \times 71.7)/0.121 = 177.8\ \text{kg m}^{-2}\text{s}^{-1}$

Velocity $= 177.8/520 = 0.34\ \text{m/s}$

$$\text{Re}_L = \frac{520 \times 0.34 \times 25 \times 10^{-3}}{0.12 \times 10^{-3}} = 36,833$$

From Fig. 19.23 $j_h = 3.3 \times 10^{-3}$:

$$\text{Nu} = 3.3 \times 10^{-3} \times 36,833 \times 2.78^{0.33} = 170.3$$
$$h_i = 170.3 \times \left(0.12/25 \times 10^{-3}\right) = 817 \text{ W/m}^{2\circ}\text{C} \quad (19.15)$$

again, neglecting the viscosity correction factor.

From Fig. 19.52, the convective boiling factor, $f_c = 3.6$:

$$\text{Re}_L \times f_c^{1.25} = 36,883 \times 3.6^{1.25} = 182,896\left(1.8 \times 10^{-5}\right)$$

From Fig. 19.53 the nucleate boiling suppression factor, $f_s = 0.23$.

So, $$h_{cb} = 3.6 \times 817 + 0.23 \times 4083 = 3880 \text{ W/m}^{2^\circ}\text{C}$$

This value has been calculated at the outlet conditions.
Assuming that the coefficient changes linearly from the inlet to outlet, then the average coefficient will be given by:

$$[\text{inlet coefficient (all liquid)} + \text{outlet coefficient (liquid} + \text{vapor)}]/2$$

$$\text{Re}_L \text{ at inlet} = 36,833 \times 0.4/0.3 = 49,111 \left(4.9 \times 10^{-4}\right)$$

From Fig. 19.23, $j_h = 3.2 \times 10^{-3}$

$$\text{Nu} = 3.2 \times 10^{-3} \times 49,111 \times 2.78^{0.33} = 220.2$$
$$h_i = 220.2 \times \left(0.12/25 \times 10^{-3}\right) = 1057 \text{ W/m}^{2\circ}\text{C}$$

Mean coefficient $= (1057 + 3880)/2 = \underline{\underline{2467}}$ $\text{Wm}^{-2^\circ}\text{C}^{-1}$

The overall coefficient, U, neglecting the resistance of the tube wall and taking the steam coefficient as 8000 $\text{W/m}^{2^\circ}\text{C}$, is given by:

$$1/U = 1/8000 + 1/2467 = 5.30 \times 10^{-4}$$
$$U = \underline{\underline{1886}} \text{ Wm}^{-2^\circ}\text{C}^{-1}$$

The overall coefficient required for the design = duty/ΔT_{LM}
ΔT_{LM} = 158.8 - 120 = 38.8 °C, taking both streams as isothermal
So, U required = 37,900/38.3 = $\underline{\underline{990}}$ $\text{Wm}^{-2^\circ}\text{C}^{-1}$
So the area available in the proposed design is more than adequate and will take care of any fouling.
The analysis could be improved by dividing the tube length into sections, calculating the heat transfer coefficient and pressure drop over each section, and totaling. More accurate, but more complex, methods could be used to predict the two-phase pressure drop and heat transfer coefficients. The pressure drop over the inlet and outlet pipes could also be estimated, taking into account the bends and expansions and contractions. An allowance could also be included for the energy (pressure drop) required to accelerate the liquid–vapor mixture as the liquid is vaporized. This can be taken as two velocity head, based on the mean density.

19.11.6 Design of kettle reboilers

Kettle reboilers and other submerged bundle equipment are essentially pool-boiling devices, and their design is based on data for nucleate boiling.

In a tube bundle, the vapor rising from the lower rows of tubes passes over the upper rows. This has two opposing effects: there will be a tendency for the rising vapor to blanket the upper tubes, particularly if the tube spacing is close, which will reduce the heat transfer rate, but this is offset by the increased turbulence caused by the rising vapor bubbles. Palen and Small (1964) give a detailed procedure for kettle reboiler design in which the heat transfer coefficient calculated using equations for boiling on a single tube is reduced by an empirically derived tube bundle factor to account for the effects of vapor blanketing. Later work by HTRI reported by Palen et al. (1972), showed that the coefficient for bundles was usually greater than that estimated for a single tube. On balance, it seems reasonable to use the correlations for single tubes to estimate the coefficient for tube bundles without applying any correction (Equations 19.41 and 19.42).

The maximum heat flux for stable nucleate boiling will, however, be less for a tube bundle than for a single tube. Palen and Small (1964) suggest modifying the Zuber equation for single tubes (Equation 19.43) with a tube density factor. This approach was supported by Palen et al. (1972).

The modified Zuber equation can be written as:

$$q_{cb} = K_b \left(\frac{p_t}{d_o}\right)\left(\frac{\lambda}{\sqrt{N_t}}\right)\left[\sigma g(\rho_L - \rho_v)\rho_v^2\right]^{0.25} \tag{19.52}$$

where q_{cb} = maximum (critical) heat flux for the tube bundle, W/m^2
K_b = 0.44 for square pitch arrangements
= 0.41 for equilateral triangular pitch arrangements
p_t = tube pitch
d_o = tube outside diameter
N_t = total number of tubes in the bundle

Note. For U-tubes, N_t will be equal to twice the number of actual U-tubes.

Palen and Small suggest that a factor of safety of 0.7 be applied to the maximum flux estimated from Equation 19.52. This will still give values that are well above those that have traditionally been used for the design of commercial kettle reboilers, such as that of 37,900 W/m^2 (12,000 Btu/ft^{2}h) recommended by Kern (1950). This has had important implications in the application of submerged bundle reboilers, as the high heat flux allows a smaller bundle to be used, which can then often be installed in the base of the column, saving the cost of shell and piping.

General design considerations

A typical layout is shown in Fig. 19.8. The tube arrangement, triangular or square pitch, will not have a significant effect on the heat transfer coefficient. A tube pitch of between 1.5 and 2.0 times the tube outside diameter should be used to avoid vapor blanketing. Long, thin bundles will be more efficient than short, fat bundles.

The shell should be sized to give adequate space for the disengagement of the vapor and liquid. The shell diameter required will depend on the heat flux. The following values can be used as a guide:

Heat flux W/m^2	Shell dia./bundle dia.
25,000	1.2– 1.5
25,000–40,000	1.4–1.8
40,000	1.7–2.0

The freeboard between the liquid level and shell should be at least 0.25 m. To avoid excessive entrainment, the maximum vapor velocity $\hat{u}_v$ (m/s) at the liquid surface should be less than that given by the expression:

$$\hat{u}_v < 0.2\left[\frac{\rho_L - \rho_v}{\rho_v}\right]^{1/2} \tag{19.53}$$

When only a low rate of vaporization is required, a vertical cylindrical vessel with a heating jacket or coils should be considered. The boiling coefficients for internal submerged coils can be estimated using the equations for nucleate pool boiling.

Mean temperature differences

When the fluid being vaporized is a single component and the heating medium is steam (or another condensing vapor), both shell- and tube-side processes are isothermal and the mean temperature difference will be simply the difference between the saturation temperatures. If one side is not isothermal, the logarithmic mean temperature difference should be used. If the temperature varies on both sides, the logarithmic temperature difference must be corrected for departures from true cross-current or countercurrent flow (see Section 19.6).

If the feed is subcooled, the mean temperature difference should still be based on the boiling point of the liquid, as the feed will rapidly mix with the boiling pool of liquid; the quantity of heat required to bring the feed to its boiling point must be included in the total duty.

Mixtures

The equations for estimating nucleate boiling coefficients given in Section 19.11.1 can be used for close boiling mixtures, say less than 5 °C, but will overestimate the coefficient if used for mixtures with a wide boiling range. Palen and Small (1964) give an empirical correction factor for mixtures that can be used to estimate the heat transfer coefficient in the absence of experimental data:

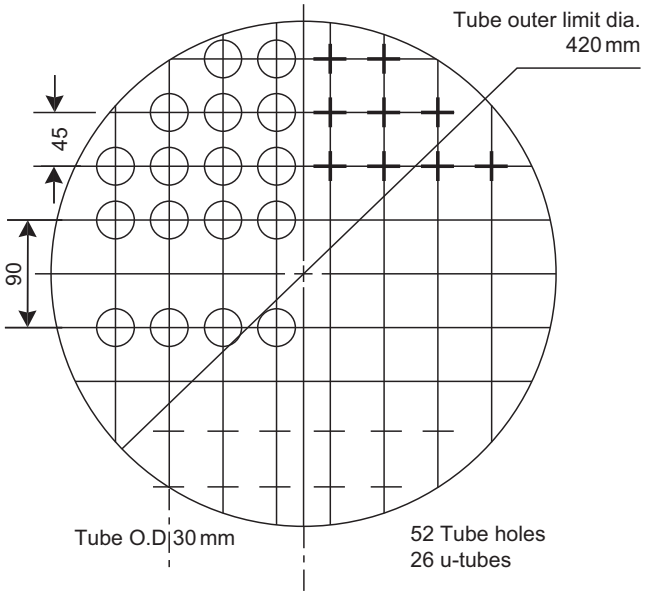
$$(h_{nb}) \text{ mixture} = f_m(h_{nb}) \text{ single component} \tag{19.54}$$

where $f_m = \exp[-0.0083(T_{bo} - T_{bi})]$
and T_{bo} = temperature of the vapor mixture leaving the reboiler °C
T_{bi} = temperature of the liquid entering the reboiler °C

The inlet temperature is the saturation temperature of the liquid at the base of the column, and the vapor temperature is the saturation temperature of the vapor returned to the column. The composition of these streams will be fixed by the distillation column design specification.

Example 19.12

Design a vaporizer to vaporize 5000 kg/h n-butane at 5.84 bar. The minimum temperature of the feed (winter conditions) will be 0 °C. Steam is available at 1.70 bar (10 psig).



Tube sheet layout, U-tubes, Example 19.12.

Solution

Only the thermal design and general layout will be done. Select kettle type.
Physical properties of n-butane at 5.84 bar:

boiling point = 56.1 °C
latent heat = 326 kJ/kg
mean specific heat, liquid = 2.51 kJ/kg°C
critical pressure, P_c = 38 bar

Heat loads:

$$\text{sensible heat(maximum)} = (56.1 - 0)2.51 = 140.8 \text{ kJ/kg}$$

$$\text{total heat load} = (140.8 + 326) \times \frac{5000}{3600} = 648.3 \text{ kW}$$

add 5 % for heat losses

$$\text{maximum heat load(duty)} = 1.05 \times 648.3$$

$$= 681 \text{ kW}$$

From Fig. 19.1, assume $U = 1000$ W/m$^{2^\circ}$C.
Mean temperature difference; both sides isothermal, steam saturation temperature at 1.7 bar = 115.2 °C

$$\Delta T_m = 115.2 - 56.1 = 59.1^\circ\text{C}$$

$$\text{Area (outside) required} = \frac{681 \times 10^3}{1000 \times 59.1} = 11.5 \text{ m}^2$$

Select 25 mm i.d., 30 mm o.d. plain U-tubes:

$$\text{Nominal length } 4.8 \text{ m(one U} - \text{tube)}$$

$$\text{Number of U tubes} = \frac{11.5}{(30 \times 10^{-3})\pi 4.8} = 25$$

Use square pitch arrangement, pitch = 1.5 × tube o.d.

$$= 1.5 \times 30 = 45 \text{ mm}$$

Draw a tube layout diagram; take minimum bend radius:

$$1.5 \times \text{tube o.d.} = 45 \text{ mm}$$

Proposed layout gives 26 U-tubes, tube outer limit diameter 420 mm.

Boiling coefficient

Use Mostinski's equation. Heat flux, based on estimated area:

$$q = \frac{681}{11.5} = 59.2 \text{ kW/m}^2$$

$$h_{nb} = 0.104(38)^{0.69}(59.2 \times 10^3)^{0.7}\left[1.8\left(\frac{5.84}{38}\right)^{0.17} + 4\left(\frac{5.84}{38}\right)^{1.2} + 10\left(\frac{5.84}{38}\right)^{10}\right] \tag{19.42}$$

$$= 4855 \text{ W/m}^{2^\circ}\text{C}$$

Take steam condensing coefficient as 8000 W/m$^{2\circ}$C, fouling coefficient 5000 W/m$^{2\circ}$C; butane fouling coefficient, essentially clean, 10,000 W/m$^{2\circ}$C. Tube material will be plain carbon steel, $k_w = 55$ W/m°C.

$$\frac{1}{U_o} = \frac{1}{4855} + \frac{1}{10,000} + \frac{30 \times 10^{-3} \ln\frac{30}{25}}{2 \times 55} + \frac{30}{25}\left(\frac{1}{5000} + \frac{1}{8000}\right) \tag{19.2}$$

$$U_o = \underline{\underline{1341}} \text{ W/m}^{2^\circ}\text{C}$$

Close enough to original estimate of 1000 W/m$^{2\circ}$C for the design to stand.
Myers and Katz (1953) give some data on the boiling of n-butane on banks of tubes. To compare the value estimated with their values, an estimate of the boiling film temperature difference is required:

$$= \frac{1341}{4855} \times 59.1 = 16.3^\circ\text{C } (29^\circ\text{F})$$

Myers data, extrapolated, gives a coefficient of around 3000 Btu/h ft^2 °F at a 29 °F temperature difference = 17,100 W/m^2°C, so the estimated value of 4855 is certainly on the safe side.

Check the maximum allowable heat flux. Use the modified Zuber equation.

$$\text{Surface tension (estimated)} = 9.7 \times 10^{-3}\text{N/m}$$

$$\rho_L = 550 \text{ kg/m}^3$$

$$\rho_v = \frac{58}{22.4} \times \frac{273}{(273+56)} \times 5.84 = 12.6 \text{ kg/m}^3$$

$$N_t = 52$$

For square arrangement $K_b = 0.44$:

$$q_c = 0.44 \times 1.5 \times \frac{326 \times 10^3}{\sqrt{52}} \left[9.7 \times 10^{-3} \times 9.81(550 - 12.6)12.6^2\right]^{0.25} \tag{19.52}$$

$$= 283,224 \text{ W/m}^2$$

$$= 280 \text{ kW/m}^2$$

Applying a factor of 0.7, maximum flux should not exceed 280 × 0.7 = 196 kW/m^2. Actual flux of 59.2 kW/m^2 is well below maximum allowable.

Layout

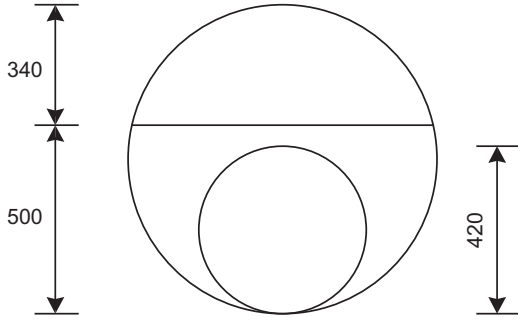
From the tubesheet layout, $D_b = 420$ mm.

Take shell diameter as twice bundle diameter:

$$D_s = 2 \times 420 = 840 \text{ mm}$$

Take liquid level as 500 mm from base:

$$\text{freeboard} = 840 - 500 = 340 \text{ mm, satisfactory.}$$



From sketch, width at liquid level = 0.8 m.

Surface area of liquid = 0.8 × 2.4 = 1.9 m^2.

$$\text{Vapor velocity at surface} = \frac{5000}{3600} \times \frac{1}{12.6} \times \frac{1}{1.9} = \underline{\underline{0.06 \text{ m/s}}}$$

Maximum allowable velocity:

$$\hat{u}_v = 0.2\left[\frac{550 - 12.6}{12.6}\right]^{1/2} = \underline{\underline{1.3}} \text{ m/s} \tag{19.53}$$

So actual velocity is well below maximum allowable velocity. A smaller shell diameter could be considered.

19.12 Plate heat exchangers

19.12.1 Gasketed plate heat exchangers

A gasketed plate heat exchanger consists of a stack of closely spaced thin plates clamped together in a frame. A thin gasket seals the plates around their edges. The plates are normally between 0.5 and 3 mm thick, and the gap between them is 1.5 to 5 mm. Plate surface areas range from 0.03 to 1.5 m^2, with a plate width:length ratio from 2.0 to 3.0. The size of plate heat exchangers can vary from very small, 0.03 m^2, to very large, 1500 m^2. The maximum flow rate of fluid is limited to around 2500 m^3/h.

The basic layout and flow arrangement for a gasketed plate heat exchanger are shown in Fig. 19.56. Corner ports in the plates direct the flow from plate to plate. The plates are embossed with a pattern of ridges, which increase the rigidity of the plate and improve the heat transfer performance.

Plates are available in a wide range of metals and alloys, including stainless steel, aluminum, and titanium. A variety of gasket materials can be used (Table 19.7).

Selection

The advantages and disadvantages of gasketed plate heat exchangers compared with conventional shell and tube exchangers are listed next:

Advantages:

1. Plates are attractive when material costs are high.
2. Plate heat exchangers are easier to maintain.
3. Low approach temperatures can be used, as low as 1 °C, compared with 5 °C to 10 °C for shell and tube exchangers.
4. Plate heat exchangers are more flexible; it is easy to add extra plates.
5. Plate heat exchangers are more suitable for highly viscous materials.
6. The temperature correction factor, F_t, will normally be higher with plate heat exchangers, as the flow is closer to true countercurrent flow.
7. Fouling tends to be significantly less in plate heat exchangers (Table 19.8).

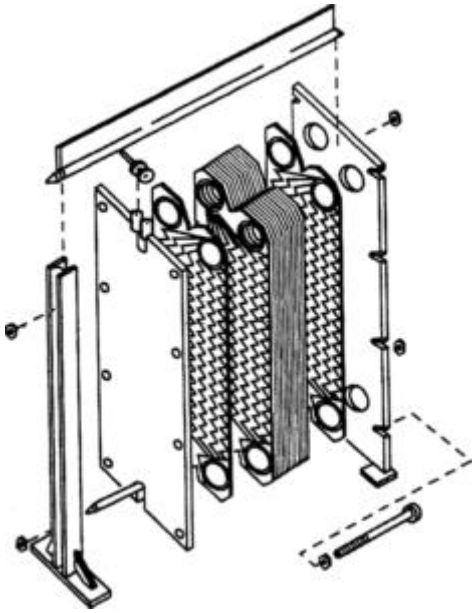


FIG. 19.56 Gasketed plate heat exchanger.

Disadvantages:

1. A plate is not a good shape to resist pressure, and plate heat exchangers are not suitable for pressures greater than about 30 bar or for high differential pressures between the two streams transferring heat.
2. The selection of a suitable gasket is critical; see Table 19.7.
3. The maximum operating temperature is limited to about 250 °C due to the performance of the available gasket materials.

Plate heat exchangers are used extensively in the food and beverage industries, as they can be readily taken apart for cleaning and inspection. Their use in the chemical industry depends on the relative cost for the particular application compared with a conventional shell and tube exchanger; see Parker (1964) and Trom (1990).

TABLE 19.7 Typical gasket materials for plated heat exchangers

Material	Approximate temperature limit, °C	Fluids
Styrene–butane rubber	85	Aqueous systems
Acrylonitrile–butane rubber	140	Aqueous system, fats, aliphatic hydrocarbons
Ethylene–propylene rubber	150	Wide range of chemicals
Fluorocarbon rubber	175	Oils
Compressed asbestos	250	General resistance to organic chemicals

TABLE 19.8 Fouling factors (coefficients), typical values for plate heat exchangers

Fluid	Coefficient ($W/m^2°C$)	Factor ($m^2°C/W$)
Process water	30,000	0.00003
Towns water (soft)	15,000	0.00007
Towns water (hard)	6000	0.00017
Cooling water (treated)	8000	0.00012
Sea water	6000	0.00017
Lubricating oil	6000	0.00017
Light organics	10,000	0.0001
Process fluids	5000–20,000	0.0002–0.00005

Plate heat exchanger design

It is not possible to give exact design methods for plate heat exchangers. They are proprietary designs and are normally specified in consultation with the manufacturers. Information on the performance of the various patterns of plate used is not generally available. Emerson (1967) gives performance data for some proprietary designs, and Kumar (1984) and Bond (1981) have published design data for APV chevron patterned plates.

The approximate method given next can be used to size an exchanger for comparison with a shell and tube exchanger and to check performance of an existing exchanger for new duties. More detailed design methods are given by Hewitt et al. (1994) and Cooper and Usher (1983).

Procedure:

The design procedure is similar to that for shell and tube exchangers.

1. Calculate duty, the rate of heat transfer required.
2. If the specification is incomplete, determine the unknown fluid temperature or fluid flow rate from a heat balance.
3. Calculate the log mean temperature difference, ΔT_{lm}.
4. Determine the log mean temperature correction factor, F_t; see the method given later.

5. Calculate the corrected mean temperature difference $\Delta T_m = F_t \times \Delta T_{lm}$.
6. Estimate the overall heat transfer coefficient; see Table 19.1.
7. Calculate the surface area required; see Equation 19.1.
8. Determine the number of plates required = total surface area/area of one plate.
9. Decide the flow arrangement and number of passes.
10. Calculate the film heat transfer coefficients for each stream; see the method given later.
11. Calculate the overall coefficient, allowing for fouling factors.
12. Compare the calculated with the assumed overall coefficient. If satisfactory, say −0% to +10% error, proceed. If unsatisfactory, return to step 8 and increase or decrease the number of plates.
13. Check the pressure drop for each stream; see method given later.

This design procedure is illustrated in Example 19.13.

Flow arrangements

The stream flows can be arranged in series or parallel, or a combination of series and parallel, (Fig. 19.57). Each stream can be subdivided into a number of passes, analogous to the passes used in shell and tube exchangers.

Estimation of the temperature correction factor

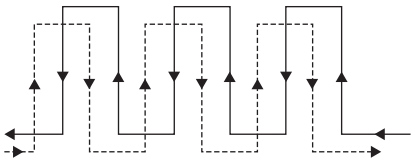
For plate heat exchangers, it is convenient to express the log mean temperature difference correction factor, F_t, as a function of the number of transfer units, *NTU*, and the flow arrangement (number of passes) (Fig. 19.58). The correction will normally be higher for a plate heat exchanger than for a shell and tube exchanger operating with the same temperatures. For rough sizing purposes, the factor can be taken as 0.95 for series flow.

The number of transfer units is given by:

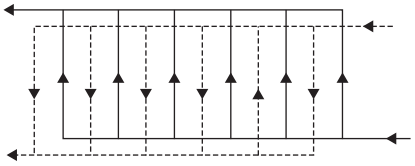
$$NTU = (t_o - t_i)/\Delta T_{lm} \tag{19.55}$$

where t_i = stream inlet temperature, °C
t_o = stream outlet temperature, °C
ΔT_{lm} = log mean temperature difference, °C

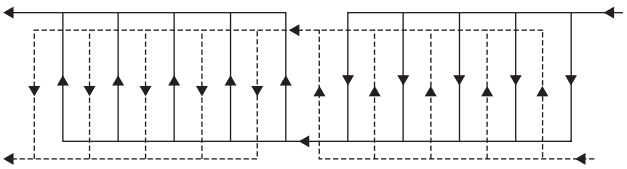
Typically, the *NTU* will range from 0.5 to 4.0, and for most applications will lie between 2.0 and 3.0.



(a) Series flow



(b) Looped (parallel) flow



(c) 2 pass/2 pass,
5 channels per pass,
19 thermal plates, 21 plates total
Countercurrent flow

FIG. 19.57 Plate heat-exchanger flow arrangements.

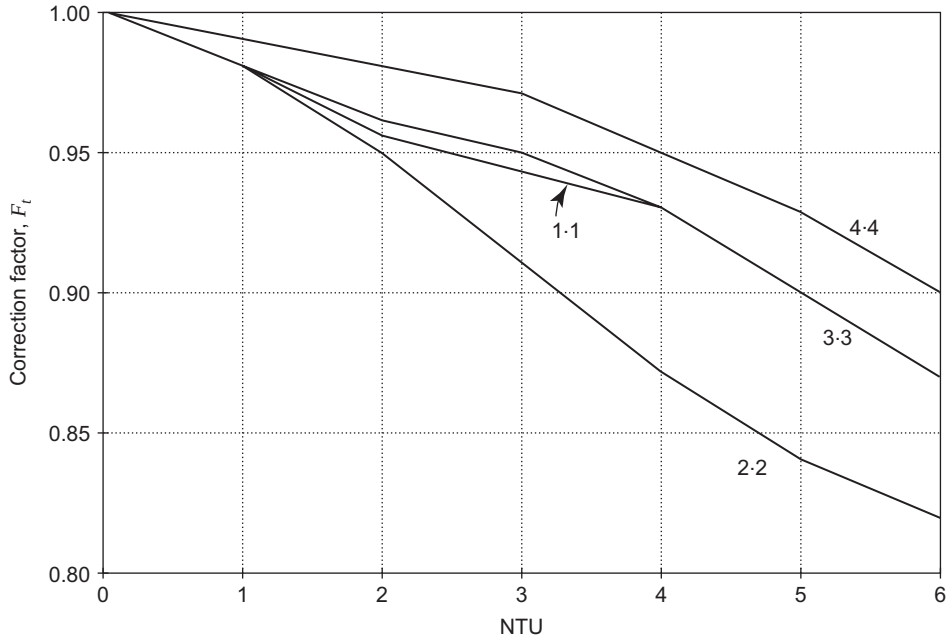


FIG. 19.58 Log mean temperature correction factor for plate heat exchangers. *Adapted from Raju & Chand 1980.*

Heat transfer coefficient

The equation for forced-convective heat transfer in conduits can be used for plate heat exchangers; see Equation 19.10.

The values for the constant C and the indices a, b, and c will depend on the particular type of plate being used. Typical values for turbulent flow are given in the following equation, which can be used to make a preliminary estimate of the area required.

$$\frac{h_p\, d_e}{k_f} = 0.26\, \mathrm{Re}^{0.65}\, \mathrm{Pr}^{0.4} \left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.56}$$

where h_p = plate film coefficient

Re = Reynolds number $= \frac{G_p d_e}{\mu} = \frac{\rho u_p d_e}{\mu}$

G_P = mass flow rate per unit cross-sectional area $= w/A_f$, $\mathrm{kgm^{-2}\ s^{-1}}$

w = mass flow rate per channel, kg/s

A_f = cross-sectional area for flow, $\mathrm{m^2}$

u_p = channel velocity, m/s

d_e = equivalent (hydraulic) diameter, taken as twice the gap between the plates, m

The corrugations on the plates will increase the projected plate area and reduce the effective gap between the plates. For rough sizing, where the actual plate design is not known, this increase can be neglected. The channel width equals the plate pitch minus the plate thickness.

There is no heat transfer across the end plates, so the number of effective plates will be the total number of plates less two.

Pressure drop

The plate pressure drop can be estimated using a form of the equation for flow in a conduit, Equation 19.18.

$$\Delta P_p = 8 j_f (L_p / d_e) \frac{\rho u_p^2}{2} \tag{19.57}$$

where L_P = the path length and $u_p = G_p/\rho$.

The value of the friction factor, j_f, depends on the design of plate used. For preliminary calculations, the following relationship can be used for turbulent flow:

$$j_f = 0.6\mathrm{Re}^{-0.3}$$

The transition from laminar to turbulent flow will normally occur at a Reynolds number of 100 to 400, depending on the plate design. With some designs, turbulence can be achieved at very low Reynolds numbers, which makes plate heat exchangers quite suitable for use with viscous fluids.

The pressure drop due to the contraction and expansion losses through the ports in the plates must be added to the friction loss. Kumar (1984) suggests adding 1.3 velocity heads per pass, based on the velocity through the ports.

$$\Delta P_{pt} = 1.3\frac{\left(\rho u_{pt}^2\right)}{2}N_p \tag{19.58}$$

where u_{pt} = the velocity through the ports $w/\rho A_p$, m/s
w = mass flow through the ports, kg/s
A_p = area of the port $= \left(\pi d_{pt}^2\right)\Big/4$,m^2
d_{pt} = port diameter, m
N_p = number of passes

Example 19.13

Investigate the use of a gasketed plate heat exchanger for the duty set out in Example 19.1: cooling methanol using brackish water as the coolant. Titanium plates are to be specified to resist corrosion by the saline water.

Summary of Example 19.1

Cool 100,000 kg/h of methanol from 95 °C to 40 °C, duty 4340 kW. Cooling water inlet temperature 25 °C and outlet temperature 40 °C. Flow rates: methanol 27.8 kg/s, water 68.9 kg/s.

Physical properties:	Methanol	Water
Density, kg/m^3	750	995
Viscosity, mN m^{-2}s	3.4	0.8
Prandtl number	5.1	5.7

Logarithmic mean temperature difference: 31 °C.

Solution

NTU, based on the maximum temperature difference:

$$= \frac{95-40}{31} = 1.8$$

Try a 1:1 pass arrangement.
From Fig. 19.58, $F_t = 0.96$
From Table 19.2, take the overall coefficient, light organic–water, to be 2000 W/m^2°C.
Then, area required

$$= \frac{4340 \times 10^3}{2000 \times 0.96 \times 31} = 72.92 \text{ m}^2$$

Select an effective plate area of 0.75 m^2, effective length 1.5 m, and width 0.5 m; these are typical plate dimensions. The actual plate size will be larger to accommodate the gasket area and ports.

$$\text{Number of plates} = \text{total heat transfer area / effective area of one plate} = 72.92/0.75 = 97$$

No need to adjust this, 97 will give an even number of channels per pass, allowing for an end plate.

$$\text{Number of channels per pass} = (97-1)/2 = 48$$

Take plate spacing as 3 mm, a typical value, then :

$$\text{Channel cross-sectional area} = 3 \times 10^{-3} \times 0.5 = 0.0015 \text{ m}^2$$

$$\text{Hydraulic mean diameter} = 2 \times 3 \times 10^{-3} = 6 \times 10^{-3} \text{ m}$$

Methanol

$$\text{Channel velocity} = \frac{27.8}{750} \times \frac{1}{0.0015} \times \frac{1}{48} = 0.51 \text{ m/s}$$

$$\text{Re} = \frac{\rho\, u_p\, d_e}{\mu} = \frac{750 \times 0.51 \times 6 \times 10^{-3}}{0.34 \times 10^{-3}} = 6750$$

$$\text{Nu} = 0.26(6750)^{0.65} \times 5.1^{0.4} = 153.8 \tag{19.56}$$

$$h_p = 153.8 \left(\frac{0.19}{6 \times 10^{-3}}\right) = 4870 \text{ Wm}^{-2^\circ}\text{C}$$

Brackish water

$$\text{Channel velocity} = \frac{68.9}{995} \times \frac{1}{0.0015} \times \frac{1}{48} = 0.96 \text{ m/s}$$

$$\text{Re} = \frac{995 \times 0.96 \times 6 \times 10^{-3}}{0.8 \times 10^{-3}} = 7164$$

$$\text{Nu} = 0.26(7164)^{0.65} \times 5.7^{0.4} = 167.2 \tag{19.56}$$

$$h_p = 167.2 \left(\frac{0.59}{6 \times 10^{-3}}\right) = 16,439 \text{ Wm}^{-2^\circ}\text{C}$$

Overall coefficient

From Table 19.2, take the fouling factors (coefficients) as brackish water (seawater) 6000 W/m$^{2^\circ}$C and methanol (light organic) 10,000 W/m$^{2^\circ}$C.

Take the plate thickness as 0.75 mm. Thermal conductivity of titanium 21 W/m°C.

$$\frac{1}{U} = \frac{1}{4870} + \frac{1}{10,000} + \frac{0.75 \times 10^{-3}}{21} + \frac{1}{16,439} + \frac{1}{6000}$$

$U = 1759$ W/m$^{2^\circ}$C, too low

Increase the number of channels per pass to 60, giving $(2 \times 60) + 1 = 121$ plates.
Then, methanol channel velocity $= 0.51 \times (48/60) = 0.41$ m/s and Re = 5400.
Cooling water channel velocity $= 0.96 \times (48/60) = 0.77$ m/s and Re = 5746.
Giving $h_p = 4215$ W/m$^{2^\circ}$C for methanol and 14,244 W/m$^{2^\circ}$C for water.
Which gives an overall coefficient of 1640 W/m$^{2^\circ}$C.
Overall coefficient required $2000 \times 48/60 = \underline{\underline{1600}}$ Wm$^{-2^\circ}$C^{-1}, so 60 plates per pass should be satisfactory.

Pressure drops

Methanol:

$$j_f = 0.60(5400)^{-0.3} = 0.046$$

Path length = plate length × number of passes = 1.5 × 1 = 1.5 m.

$$\Delta P_p = 8 \times 0.046\left(\frac{1.5}{6 \times 10^{-3}}\right) \times 750 \times \frac{0.41^2}{2} = 5799 \text{ N/m}^2 \tag{19.57}$$

Port pressure loss, take port diameter as 100 mm, area = 0.00785 m^2.

Velocity through port = (27.8/750)/0.00785 = 4.72 m/s.

$$\Delta P_{pt} = 1.3 \times \frac{750 \times 4.72^2}{2} = 10,860 \text{ N/m}^2 \tag{19.58}$$

Total pressure drop = 5799 + 10,860 = $\underline{\underline{16,659}}$ N/m^2, 0.16 bar.

Water:

$$j_f = 0.6(5501)^{-0.3} = 0.045$$

Path length = plate length × number of passes = 1.5 × 1 = 1.5 m.

$$\Delta P_p = 8 \times 0.045 \times \left(\frac{1.5}{6 \times 10^{-3}}\right) \times 995 \times \frac{0.77^2}{2} = 26,547 \text{ N/m}^2 \tag{19.57}$$

Velocity through port = (68.9/995)/0.0078 = 8.88 m/s (rather high)

$$\Delta P_{pt} = 1.3 \times \frac{995 \times 8.88}{2} = 50,999 \text{ N/m}^2$$

Total pressure drop = 26,547 + 50,999 = $\underline{\underline{77,546}}$ N/m^2, 0.78 bar

Could increase the port diameter to reduce the pressure drop.

The trial design should be satisfactory, so a plate heat exchanger could be considered for this duty.

19.12.2 Welded plate exchangers

Welded plate heat exchangers use plates similar to those in gasketed plate exchangers, but the plate edges are sealed by welding. This increases the pressure and temperature rating to up to 80 bar and temperatures in excess of 500 °C. They retain the advantages of plate heat exchangers (compact size and good rates of heat transfer) while giving security against leakage. An obvious disadvantage is that the exchangers cannot be dismantled for cleaning, so their use is restricted to applications where fouling is not a problem. The plates are fabricated in a variety of materials.

A welded plate exchanger can be specified for a high-pressure service if it is contained inside a pressure vessel and the space between the exchanger and the vessel is pressurized to the same pressure as the fluid inside the exchanger. The differential pressure between the two sides of the exchanger must still be small.

A combination of gasketed and welded plate construction can also be used, with an aggressive process fluid flowing between welded plates and a benign process stream, or service stream, between gasketed plates.

19.12.3 Plate-fin exchangers

Plate-fin exchangers consist essentially of plates separated by corrugated sheets, which form the fins. They are made up in a block and are often referred to as matrix exchangers (Fig. 19.59). They are usually constructed of aluminum and joined and sealed by brazing. The main application of plate-fin exchangers has been in the cryogenics industries, such as air separation plants, where large heat transfer surface areas are needed. They are now finding wider applications in the chemical process industries, in applications where large surface area, compact, exchangers are required. Their compact size and low weight have led to some use in offshore applications. The brazed

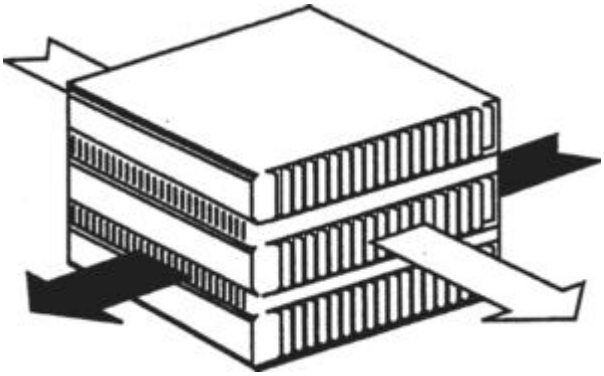


FIG. 19.59 Plate-fin exchanger.

aluminum construction is limited to pressures up to around 60 bar and temperatures up to 150 °C. The units cannot be mechanically cleaned, so their use is restricted to clean process and service steams. The construction and design of plate-fin exchangers and their applications are discussed by Saunders (1988) and Burley (1991) and their use in cryogenic service by Lowe (1987).

19.12.4 Spiral heat exchangers

A spiral heat exchanger can be considered as a plate heat exchanger in which the plates are formed into a spiral. The fluids flow through the channels formed between the plates. The exchanger is made up of long sheets, between 150 and 1800 mm wide, formed into a pair of concentric spiral channels. The channels are closed by gasketed end plates bolted to an outer case. Inlet and outlet nozzles are fitted to the case and connect to the channels (Fig. 19.60). The gap between the sheets varies between 4 and 20 mm; depending on the size of the exchanger and the application. They can be fabricated in any material that can be cold-worked and welded.

Spiral heat exchangers are compact units: a unit with around 250 m^2 area occupying a volume of approximately 10 m^3. The maximum operating pressure is limited to 20 bar and the temperature to 400 °C.

For a given duty, the pressure drop over a spiral heat exchanger will usually be lower than that for the equivalent shell and tube exchanger. Spiral heat exchangers give true countercurrent flow and can be used where the temperature correction factor F_t for a shell and tube exchanger would be too low; see Section 19.6. Because they are easily cleaned and the turbulence in the channels is high, spiral heat exchangers can be used for very dirty process fluids and slurries.

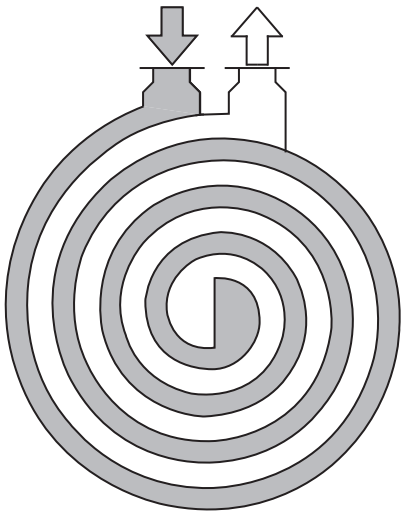


FIG. 19.60 Spiral heat exchanger.

The correlations for flow in conduits can be used to estimate the heat transfer coefficient and pressure drop in the channels, using the hydraulic mean diameter as the characteristic dimension.

The design of spiral heat exchangers is discussed by Minton (1970).

19.13 Direct-contact heat exchangers

In direct-contact heat exchange the hot and cold streams are brought into contact without any separating wall, and high rates of heat transfer are achieved. Applications include reactor off-gas quenching, vacuum condensers, cooler-condensers, desuperheating, and humidification. Water cooling towers are a particular example of direct-contact heat exchange; see Section 3.2.5. In direct-contact cooler-condensers, the condensed liquid is frequently used as the coolant (Fig. 19.61).

Direct-contact heat exchangers should be considered whenever the process stream and coolant are compatible. The equipment used is simple and cheap and is suitable for use with heavily fouling fluids and with liquids containing solids; spray chambers, spray columns, and plate and packed columns are used.

There is no general design method for direct-contact exchangers. Most applications involve the transfer of latent heat as well as sensible heat, and the process is one of simultaneous heat and mass transfer. When the approach to thermal equilibrium is rapid, as it will be in many applications, the size of the contacting vessel is not critical and the design can be based on experience with similar processes. For other situations, the designer must work from first principles, setting up the differential equations for mass and heat transfer and using judgment in making the simplifications necessary to achieve a solution. The design procedures used are analogous to those for gas absorption and distillation. The rates of heat transfer will be high, with coefficients for packed columns typically in the range of 2000 to 20,000 $W/m^3{}^\circ C$ (i.e., per cubic meter of packing).

The design and application of direct-contact heat exchangers is discussed by Fair (1961, 1972*a*, 1972*b*) and Chen-Chia and Fair (1989). They give practical design methods and data for a range of applications.

The design of water cooling towers and humidification is discussed by Chhabra and Shankar (2017). The same principles apply to the design of other direct-contact exchangers.

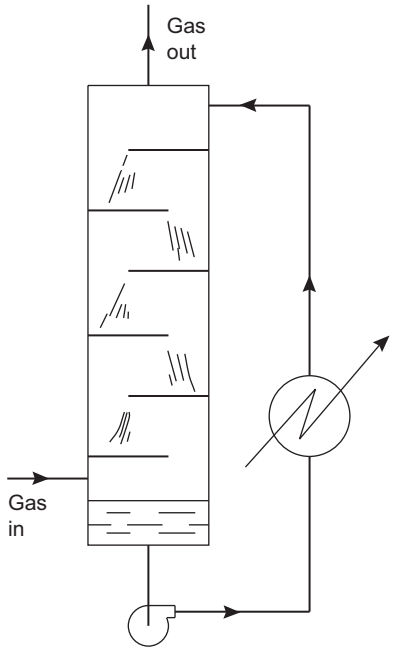


FIG. 19.61 Typical direct-contact cooler (baffle plates).

19.14 Finned tubes

Fins are used to increase the effective surface area of heat exchanger tubing. Many different types of fins have been developed, but the plain transverse fin shown in Fig. 19.62 is the most commonly used type for process heat

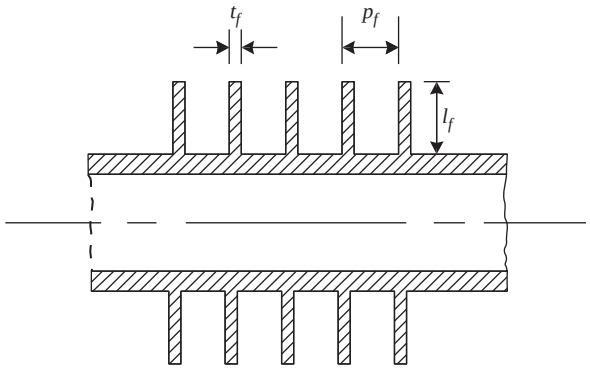


FIG. 19.62 Finned tube.

exchangers. Typical fin dimensions are pitch 2.0 to 4.0 mm, height 12 to 16 mm, and ratio of fin area to bare tube area 15:1 to 20:1.

Finned tubes are used when the heat transfer coefficient on the outside of the tube is appreciably lower than that on the inside, as in heat transfer from a liquid to a gas, such as in air-cooled heat exchangers.

The fin surface area will not be as effective as the bare tube surface, as the heat has to be conducted along the fin. This is allowed for in design by the use of a fin effectiveness, or fin efficiency, factor. The equations describing heat transfer from a fin are derived in Chhabra and Shankar (2017); see also Kern (1950). The fin effectiveness is a function of the fin dimensions and the thermal conductivity of the fin material. Fins are therefore usually made from metals with a high thermal conductivity; for copper and aluminum, the effectiveness is typically between 0.9 and 0.95.

When using finned tubes, the coefficients for the outside of the tube in Equation 19.2 are replaced by a term involving fin area and effectiveness:

$$\frac{1}{h_o}+\frac{1}{h_{od}}=\frac{1}{E_f}\left(\frac{1}{h_f}+\frac{1}{h_{df}}\right)\frac{A_o}{A_f} \tag{19.59}$$

where h_f = heat transfer coefficient based on the fin area
h_{df} = fouling coefficient based on the fin area
A_o = outside area of the bare tube
A_f = fin area
E_f = fin effectiveness

It is not possible to give a general correlation for the coefficient h_f covering all types of fins and fin dimensions. Design data should be obtained from the tube manufacturers for the particular type of tube to be used. For banks of tubes in cross flow with plain transverse fins, the correlation given by Briggs and Young (1963) can be used to make an approximate estimate of the fin coefficient.

$$\mathrm{Nu} = 0.134\,\mathrm{Re}^{0.681}\,\mathrm{Pr}^{0.33}\left(\frac{p_f - t_f}{l_f}\right)^{0.2}\left(\frac{p_f}{t_f}\right)^{0.1134} \tag{19.60}$$

where p_f = fin pitch
l_f = fin height
t_f = fin thickness

The Reynolds number is evaluated for the bare tube (i.e., assuming that no fins exist).

Kern and Kraus (1972) give full details of the use of finned tubes in process heat exchanger design and design methods.

Low fin tubes

Tubes with low transverse fins, about 1 mm high, can be used with advantage as replacements for plain tubes in many applications. The fins are formed by rolling, and the tube outside diameters are the same as those for standard plain tubes. Details are given in the manufacturer's data books, Wolverine (1984), and an electronic version of their design manual, www.wlv.com; see also Webber (1960).

19.15 Double-pipe heat exchangers

One of the simplest and cheapest types of heat exchanger is the concentric pipe arrangement shown in Fig. 19.63. These can be made up from standard pipe fittings and are useful when only a small heat transfer area is required. Several units can be connected in series to extend their capacity.

The correlation for forced convective heat transfer in conduits (Equation 19.10) can be used to predict the heat transfer coefficient in the annulus, using the appropriate equivalent diameter:

$$d_e = \frac{4 \times \text{cross-sectional area}}{\text{wetted perimeter}} = \frac{4\left(d_2^2 - d_1^2\right)\frac{\pi}{4}}{\pi(d_2 + d_1)} = d_2 - d_1$$

where d_2 is the inside diameter of the outer pipe and d_1 the outside diameter of the inner pipe. Some designs of double-pipe exchanger use inner tubes fitted with longitudinal fins.

A variant of the double-pipe heat exchanger is the hairpin exchanger shown in Fig. 19.64. A hairpin exchanger is formed by inserting one or more U-tubes into two pipe sections welded to a large flanged end, which is then closed using a removable bonnet. Each straight section of the U-tubes acts as a double-pipe exchanger. True countercurrent flow is obtained if a single U-tube is used.

Hairpin exchangers are cheaper than shell and tube exchangers at very small sizes and can be specified for areas from 7 m^2 to 150 m^2.

19.16 Air-cooled exchangers

Air-cooled exchangers consist of banks of finned tubes over which air is blown or drawn by fans mounted below or above the tubes (forced or induced draft). Typical designs are shown in Fig. 19.65.

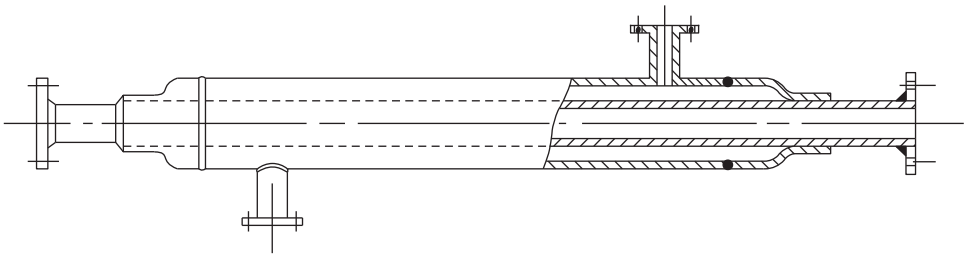


FIG. 19.63 Double-pipe exchanger (constructed for weld fittings).

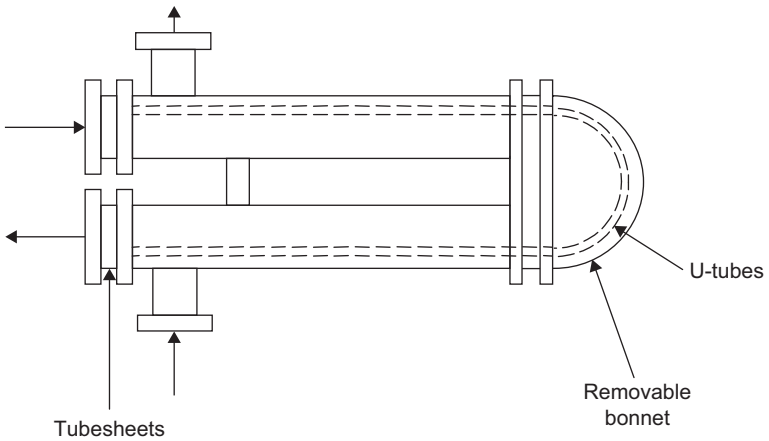


FIG. 19.64 Hairpin exchanger.

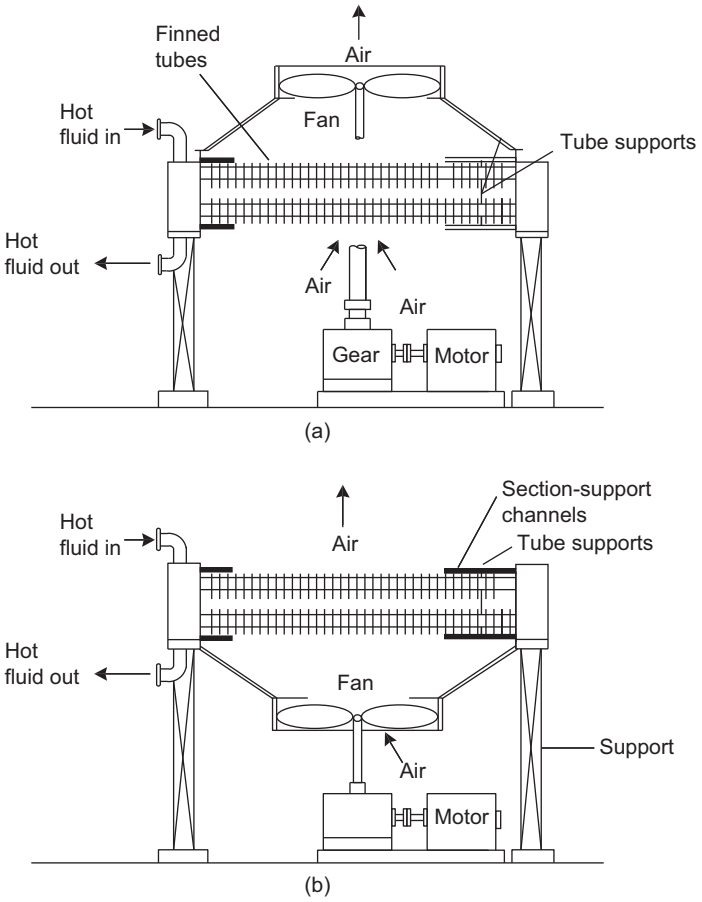


FIG. 19.65 Air-cooled exchangers. (a) Induced draft. (b) Forced draft.

Air-cooled exchangers should be considered when cooling water is in short supply or expensive. They can be competitive with water-cooled units even when water is plentiful. Frank (1978) suggests that in moderate climates air cooling will usually be the best choice for minimum process temperatures above 65 °C and water cooling for minimum processes temperatures below 50 °C. Between these temperatures a detailed economic analysis must be carried out to decide the best coolant. Air-cooled exchangers are used for cooling and condensing.

Cooling water circuits require a humidity driving force to achieve cooling of the water; see Section 3.2.5 and Chhabra and Shankar (2017). In climates that often experience a combination of high temperature and high humidity, air cooling will usually be cheaper than water cooling. Air coolers are also often specified for revamps or additions to existing plants so as to avoid increasing the cooling tower load and obviate investments in the site utility system.

The design and application of air-cooled exchangers is discussed by Rubin (1960), Lerner (1972), Brown (1978), and Mukherjee (1997). Design procedures are also given in the books by Kern (1950), Kern and Kraus (1972), and Kroger (2004). Lerner and Brown give typical values for the overall coefficient for a range of applications and provide methods for the preliminary sizing of air-cooled heat exchangers.

Details of the construction features of air-cooled exchangers are given by Coker (2015). The construction features of air-cooled heat exchangers are covered by the American Petroleum Institute Standard, API 661, which has been adopted as the recognized international standard for air coolers, ISO 13706-1:2011.

Air-cooled exchangers are packaged units and are normally selected and specified in consultation with a manufacturer. Some typical overall coefficients are given in Table 19.1. These can be used to make an approximate estimate of the area required for a given duty. The commercial heat exchanger design programs developed by HTRI and HTFS include programs for air cooler design; see Section 19.1.

19.16.1 Air coolers: Construction details

Air coolers can be designed with the fan mounted either above or below the tube rack, as illustrated in Fig. 19.65.

In an induced draft cooler (Fig. 19.65a), the fan is mounted above the bank of tubes and air is pulled up over the tubes. The housing around the fan provides for some chimney effect, which can give better cooling when the fan is not running. This design generally has better air distribution across the tube rack and lower chance of air recirculation, but the location of the fan makes maintenance access difficult, and the tubes can become damaged during fan maintenance.

Fig. 19.65(b) shows a forced draft cooler in which the fan is mounted below the bank of tubes and air is blown up across the tube bank. The natural draft capability of this design is lower, but the fan is easier to access for maintenance. The fan draws cooler air in a forced draft design, which reduces the power requirement. Forced draft designs can also recirculate air in winter to offset the effect of lower ambient temperature. Care must be taken when designing the cooler and plant layout to ensure that unwanted air recirculation does not occur during normal operation. Forced draft coolers are usually less expensive than induced draft coolers.

The tubes used in air coolers are usually finned to provide additional surface area to compensate for the poor heat transfer coefficient on the air side. Because of the use of finned tubes, air coolers are sometimes referred to as "fin-fan coolers." The ratio of finned area to bare tube area is typically about 20:1.

The tubes are usually welded into a header at each end of the exchanger, and the tube-side flow is usually two-pass so that the inlet and outlet are at the same (front) end of the cooler. The opposite (floating) header is mounted to allow for thermal expansion of the tubes. Multiple banks of tubes may be used as long as the air-side pressure drop and fan power are not excessive. Standard tube lengths are typically used, but longer tubes up to 20 m (60 ft) can be accommodated by arranging multiple fans in parallel. The height of the tube bank above the ground must be large enough to give an inlet velocity equal to the face velocity over the tube bundle. A typical height is half of the tube length per fan.

19.16.2 Heat transfer in air coolers

The air-side heat transfer coefficient in air coolers is usually very low and dominates the overall heat transfer coefficient. If the detailed design of the finned tubes is known, then the air-side coefficient can be calculated using Equation 19.60 or a similar expression provided by the tube manufacturer. When the finned tube design is not known, the fin coefficient can be estimated using the expression given by Lohrisch (1966):

$$\mathrm{Nu} = 0.28\ \mathrm{Re}^{0.6}\mathrm{Pr}^{0.33} \tag{19.61}$$

Using typical fin dimensions of fin pitch 2.3 mm (12 fins per inch), fin length 15.9 mm, and fin thickness 0.48 mm, Equation 19.60 reduces to:

$$\mathrm{Nu} = 0.104\ \mathrm{Re}^{0.681}\mathrm{Pr}^{0.33} \tag{19.62}$$

Air coolers are typically designed for the highest temperature that will be exceeded for 40 hours per year less 4 °C (API 661). This temperature is usually about 40 °C (~104 °F). At this temperature, dry air has the properties Pr ~ 0.7, $\rho \sim 1.13\ \mathrm{kg/m^3}$, $\mu \sim 1.9 \times 10^{-5}\ \mathrm{Nm^{-2}s}$ and k ~ 0.0272 W/m°C. Using a typical tube diameter of 25.4 mm and face velocity of 2.5 m/s (500 ft/min), we obtain:

From Equation 19.61: Nu ~ 34.8, $h_f \sim 37.2$
From Equation 19.62: Nu ~ 25.2, $h_f \sim 27.0$

The fin efficiency is typically about 0.9 at these values of h_f (Lohrisch, 1966), and the ratio of finned area to bare tube area is typically 20:1. Fouling factors for air are usually quite high, and the fouling coefficient can be taken as 5000 $\mathrm{W/m^2{}^\circ C}$ (from Table 19.2). Taking the average of the values of h_f calculated earlier, equation 19.59 gives:

$$\frac{1}{h_o} + \frac{1}{h_{od}} = \frac{1}{0.9}\left(\frac{1}{32} + \frac{1}{5000}\right)\frac{1}{20} \tag{19.59}$$

$$\frac{1}{h_o} + \frac{1}{h_{od}} \approx \frac{1}{600} \tag{19.63}$$

where h_o is based on the bare tube area.

Equation 19.63 can be used with Equation 19.2 to make an initial estimate of the overall heat transfer coefficient. More accurate correlations are available in the air-cooled exchanger design programs developed by HTRI (www.HTRI.net) and HTFS. The HTFS programs are part of Aspen Technology's Aspen Engineering Suite and Honeywell's UniSim Design Suite; see Table 4.1. Equations for heat transfer to tube banks in natural convection are given by Chu (2005).

19.16.3 Air cooler design

Air-cooled exchangers are designed to give satisfactory performance under most expected climate conditions. The API 661/ISO 13706 standard recommends that for critical applications, the ambient temperature shall be the highest air temperature that is exceeded for 40 hours per year. For noncritical applications, the air temperature can be taken as the higher of:

- The highest temperature that is exceeded for 400 h/y
- The highest temperature that is exceeded for 40 h/y minus 4 °C

A small allowance on ambient temperature is usually made to provide a safety margin to compensate for recirculation, typically 2 °C to 3 °C.

The procedure for designing an air cooler is then as follows:

1. Estimate the cooling duty, including heat of condensation, if phase change occurs.
2. Collect physical property data.
3. Estimate the tube inside heat transfer coefficient and fouling coefficient. Hence calculate U using Equations 19.2 and 19.63.
4. Determine the ambient air temperature for design. Ambient temperature statistics can be found from government meteorological offices and sources such as www.weather.com. Add an allowance for recirculation.
5. Estimate ΔT_{lm}, assuming that the air-side temperature is approximately constant. Hence, estimate ΔT_m, assuming F_t is 0.9. The air-side temperature is obviously not constant and typically increases by a few °C. The low change in temperature on the air side gives a high value of R and a low value of S unless the process-side outlet temperature is very close to the air temperature. Consequently, F_t is close to 1.0 for air coolers. Assuming $F_t = 0.9$ is a conservative approximation that compensates for the error introduced by using a constant air-side temperature in calculating ΔT_{lm}.
6. Estimate the bare tube area using Equation 19.1.
7. Choose a tube diameter (typically 25.4 mm) and length (typically a multiple of 6 m or 20 ft) and determine the number of tubes required. Select the tube material of construction.
8. Decide the bundle layout. Determine the number of tubes per bank and number of banks of tubes (generally fewer than 10 banks per bundle).
9. Determine the bundle area. The tube spacing is typically 50.8 mm or 63.5 mm (2.0 in. or 2.5 in.) on a triangular pitch, but wider spacing may be used if the fin length is large. The bundle area, A_b, is given by:

$$A_b = L' p_t N_{bk} \tag{19.64}$$

where L' = effective tube length
p_t = tube pitch
N_{bk} = number of tubes per bank

10. Estimate the air-side flow rate. A typical face velocity is 2.5 m/s (500 ft/min). The air flow rate is the product of face velocity and bundle area.
11. Estimate the fan power consumption. The fan power, W_f, can be estimated as:

$$W_f = \frac{u_f A_b \Delta P_b}{\eta_f} \tag{19.65}$$

where u_f = face velocity
ΔP_b = pressure drop across the bundle
η_f = fan efficiency, typically about 0.7

In customary units, Equation 19.65 is usually written as:

$$\text{Fan power (hp)} = \left(\frac{\text{ACFM}\ \Delta P_b}{6837\ \eta_f}\right) \tag{19.65b}$$

where ACFM = air flow rate in actual cubic feet per minute and ΔP_b is in inches of water.The pressure drop across the bundle is usually very low, and a value of 150 N/m^2 (0.6 in. of water) can be used as an initial estimate.

12. Estimate the overall power consumption by allowing an additional 5% to 10% for motor efficiency.
13. Carry out a detailed simulation of the specified geometry to confirm that the heat transfer coefficients and pressure drops that have been assumed are realistic. This step is usually carried out using commercial design programs. Modify the design if necessary.
14. Determine the air cooler capital and operating costs. Modify the design as necessary to optimize the total annualized cost.

This procedure is illustrated in Example 19.14.

19.16.4 Air cooler operation and control

An intrinsic problem of air coolers is that they must be designed to perform under the warmest climate conditions and so are oversized for the current ambient temperature most of the time. This can be particularly problematic in winter, when ambient temperature may be low enough to cause precipitation of components from the process fluid or even freeze the process fluid.

Temperature control of air coolers can be accomplished by varying the air flow or bypassing some hot fluid around the exchanger, as discussed in Chapter 5 and illustrated in Fig. 5.12. Several methods are used to vary air flow:

1. Variable-speed drives can be used on the fans. These have a higher cost than single-speed fans, but give the best energy efficiency and temperature control.
2. Variable-pitch fans can be specified. Changing the fan pitch varies the air flow, and power consumption is reduced at low pitch.
3. Louvers can be used to provide a restriction in the air flow path and reduce the air rate. The louvers may be manually or automatically adjusted. The use of louvers does not reduce power consumption, and louver operation can be impeded by snow or ice, but this is the cheapest method.

In regions that experience cold winters, air flow control may not be adequate for winterization. Annex C of API 661/ISO 13706 provides guidelines on when winterization is needed and describes other winterization approaches such as internal or external air recirculation.

Example 19.14

Investigate the use of an air-cooled exchanger for the duty set out in Example 19.1. Determine the fan power consumption.

Solution

Summary of Example 19.1

Cool 100,000 kg/h of methanol from 95 °C to 40 °C, duty 4340 kW. Methanol flow rate 27.8 kg/s, density 750 kg/m^3, viscosity 0.34 mNm^{-2}s, Prandtl number 5.1, thermal conductivity 0.19 W/m°C.

Step 3: Heat transfer coefficient

Assuming a typical tube-side velocity of 1.5 m/s and selecting 25.4 mm o.d. (22.1 mm i.d.) tubes:

$$\text{Re} = \frac{\rho u d_i}{\mu} = \frac{750 \times 1.5 \times 22.1 \times 10^{-3}}{0.34 \times 10^{-3}} = 73.1 \times 10^3$$

From Equation 19.11, neglecting the viscosity correction:

$$\mathrm{Nu} = 0.023\,\mathrm{Re}^{0.8}\mathrm{Pr}^{0.33}$$

$$= 0.023\left(73.1\times 10^{3}\right)^{0.8}(5.1)^{0.33} = 306.5$$

$$\text{Hence, } h_i = 306.5 \times \left(0.19/\left(22.1\times 10^{-3}\right)\right)$$

$$= 2635\ \mathrm{W/m^{2\circ}C}$$

Because the exchanger no longer uses brine as coolant, a cheaper material of construction such as plain carbon steel can be selected. For carbon steel, the thermal conductivity, k_w, is 55 W/m°C over the range of temperature of interest.

Using the same fouling coefficient of 5000 W/m^2°C for methanol and substituting Equation 19.63 in Equation 19.2 gives:

$$\frac{1}{U_o} = \frac{1}{600} + \frac{25.4\times 10^{-3}\ \ln\left(\frac{25.4}{22.1}\right)}{2\times 55} + \frac{25.4}{22.1}\times\frac{1}{2635} + \frac{25.4}{22.1}\times\frac{1}{5000} \tag{19.2}$$

$$\frac{1}{U_o} = \frac{1}{600} + \frac{1}{31120} + \frac{1}{2292} + \frac{1}{4350}$$

From which is it clear that the air-side contribution governs the overall heat transfer coefficient, and:

$$U_o = 423\ \mathrm{W/m^{2\circ}C}$$

Step 4: Ambient temperature

If the cooler is located in the U.S. Midwest, then a reasonable initial estimate of the design air temperature is 32 °C (90 °F). The ambient temperature is obviously highly site-specific, and for many regions a product temperature specification of 40 °C would immediately rule out the use of air cooling as impractical. Adding 2 °C to allow for some recirculation gives a design temperature of 34 °C.

Step 5: Estimate ΔT_m

$$\Delta T_{lm} = \frac{(95-34)-(40-34)}{\ln\left(\frac{95-34}{40-34}\right)} = 23.7^{\circ}\mathrm{C}$$

Assuming $F_t = 0.9$,

$$\Delta T_m = 0.9\times 23.7 = 21.3^{\circ}\mathrm{C}$$

Step 6: Estimate bare tube area

$$Q = UA\Delta T_m \tag{19.1}$$

hence:

$$A = \frac{4.34\times 10^{6}}{423\times 21.3} = 481.7\ \mathrm{m^2}$$

Steps 7 and 8: Pick tubes and determine bundle layout

The area of a 6 m long, 25.4 mm o.d. (20 ft, 1 in. o.d.) tube is $\pi\times 25.4\times 10^{-3}\times 6 = 0.479$ m^2, so we require $481.7/0.479 = 1006$ tubes. If we increase tube length to 18 m (60 ft), then we need 335 tubes, which can be arranged as five banks of 67 tubes each.

Step 9: Determine bundle area

If the tube pitch is 76.2 mm (3 in.), then the bundle area is:

$$A_b = 18\times 76.2\times 10^{-3}\times 67 = 91.9\ \mathrm{m^2}$$

Step 10: Estimate air flow rate

Assuming a face velocity of 2.5 m/s, the air flow rate is $2.5\times 91.9 = 229.7$ actual m^3/s.

Steps 11 and 12: Estimate fan power and total power

From Equation 19.65, assuming 150 N/m^2 pressure drop and 70% fan efficiency, the fan power is:

$$W_f = \frac{u_f A_b \Delta P_b}{\eta_f} = \frac{2.5 \times 91.9 \times 150}{0.7} = 49.2 \text{ kW} \quad (19.65)$$

Allowing for motor efficiency of 95%, the total power consumed = 49.2/0.95 = 51.8 kW.

Note that the fan power consumed is much less than the cooling duty.

Step 13: Confirm heat transfer coefficients and pressure drop

Check tube-side heat transfer:

With 335 tubes, we have 167 tubes on one pass and 168 on the other pass. Using 168 tubes, methanol flow rate = 27.8 kg/s = 27.8/750 m^3/s = 0.037 m^3/s.

Tube inside area = π $(22.1 \times 10^{-3})^2/4 = 3.836 \times 10^{-4}$ m^2 per tube.

So, tube-side velocity = $0.037/(168 \times 3.836 \times 10^{-4}) = 0.574$ m/s.

This is less than 40% of the assumed 1.5 m/s, so we need to correct the inside heat transfer coefficient. The corrected value of h_i will be:

$$h_i = 2635 \times \left(\frac{0.574}{1.5}\right)^{0.8}$$

$$= 1222 \text{ W/m}^{2\circ}\text{C}$$

The corrected value of U_o is:

$$\frac{1}{U_o} = \frac{1}{600} + \frac{1}{31120} + \frac{25.4}{22.1} \times \frac{1}{1222} + \frac{1}{4350}$$

$$U_o = 349 \text{ W/m}^{2\circ}\text{C}$$

The area required would now be $481.7 \times (423/349) = 584$ m^2, i.e., 1220 tubes

Check air-side temperature change and ΔT_m:

Air flow rate = 229.7 m^3/s

At 34 °C, air has density 1.15 kg/m^3 and C_p ~1 kJ/kg°C.

So,

$$\text{air side temperature change} = \frac{4.34 \times 10^3}{229.7 \times 1.15 \times 1} = 16.4 \text{ °C}$$

Such a large change in temperature on the air side is clearly not acceptable with a temperature approach of 6 °C at the cold end of the exchanger. To reach an acceptable air-side temperature change, we would need at least three times the air flow calculated, which would cause a factor of three increase in the fan duty. At this point, most experienced design engineers would conclude that because of the low outlet temperature specified for the cooler, an air cooler would not be economically attractive compared with a water cooler in this service.

If water cooling was not possible, then we could consider three air coolers in parallel, each with a single bank of 150 tubes, each 18 m long. Keeping the tube pitch at 76.2 mm, the bundle area is:

$$A_b = 18 \times 76.2 \times 10^{-3} \times 150 = 205.7 \text{ m}^2 (\text{roughly } 18 \text{ m} \times 12 \text{ m})$$

Assuming a face velocity of 2.5 m/s, the air flow rate in each cooler is $2.5 \times 205.7 = 514.3$ actual m^3/s, so the total air flow is 1543 actual m^3/s, roughly three times the initial design.

$$\text{air side temperature change} = \frac{4.34 \times 10^3}{514.3 \times 3 \times 1.15 \times 1} = 2.45 \text{ °C}$$

This gives

$$R = \frac{95 - 40}{2.45} = 22.4$$

$$S = \frac{2.45}{95 - 34} = 0.040$$

From which $F_t \sim 0.95$,

$$\Delta T_{lm} = \frac{(95 - 36.5) - (40 - 34)}{\ln\left(\frac{95 - 36.5}{40 - 34}\right)} = 23.1°\text{C}$$

and

$$\Delta T_m = 0.95 \times 23.1 = 21.9°\text{C}.$$

With 3×150 tubes, we have $3 \times 75 = 225$ tubes per pass, so tube-side velocity $= 0.037/(225 \times 3.836 \times 10^{-4}) = 0.429$ m/s.

$$h_i = 2635 \times \left(\frac{0.429}{1.5}\right)^{0.8}$$

$$= 967 \text{ W/m}^{2\circ}\text{C}$$

The corrected value of U_o is:

$$\frac{1}{U_o} = \frac{1}{600} + \frac{1}{31120} + \frac{25.4}{22.1} \times \frac{1}{967} + \frac{1}{4350}$$

$$U_o = 321 \text{ W/m}^{2\circ}\text{C}$$

hence

$$A = \frac{4.34 \times 10^6}{321 \times 21.9} = 617.6 \text{ m}^2$$

The area of a 18 m long, 25.4 mm o.d. (20 ft, 1 in. o.d.) tube is 1.437 m^2, so we require $617.6/1.437 = 430$ tubes. This is less than the $3 \times 150 = 450$ tubes assumed in the design, so we now have more than the required area. We could reduce the tube count slightly and iterate towards a converged solution, but the design is probably good enough at this point. The air-side heat transfer coefficient and pressure drop should now be confirmed and the design finalized using commercial air-cooler design software.

The new fan duty for each bundle is:

$$W_f = \frac{u_f A_b \Delta P_b}{\eta_f} = \frac{2.5 \times 205.7 \times 150}{0.7} = 110.2 \text{ kW} \tag{19.65}$$

Allowing for motor efficiency of 95%, the total power consumed for all three coolers $= 3 \times 110.2/0.95 = 348$ kW.

The design generated in this example is feasible, but has high plot-space requirements, as well as a higher capital cost than the water cooler. The operating cost of running these air coolers at 0.06 $/kWh would be $348 \times 0.06 = \$20.9$/h. The cost of providing cooling water to the exchanger of Example 19.1 would be roughly $6.50/h (based on cooling water cost of $0.1/1000 gal), so the operating cost of the air cooler is also higher. An air cooler is clearly less economically attractive than a water cooler in this service and would only be considered if water costs were excessive or if there was flexibility to cool the methanol to a higher outlet temperature.

19.17 Fired heaters (furnaces and boilers)

When high temperatures and high flow rates are required, fired heaters are used. Fired heaters are directly heated by the products of combustion of a fuel. The highest temperature at which steam is used for process heating is typically about 250 °C. Circulating heating oils are used up to about 330 °C, but hot oil loops themselves require a fired heater as the primary heat source. Small vertical cylindrical fired heaters are used for duties up to 45 MW, and larger cabin furnaces are used for higher duties.

Typical applications of fired heaters are:

1. Process feed-stream heaters, such as the feed heaters for high-temperature reactors and refinery crude columns (pipe still furnaces) in which up to 60% of the feed may be vaporized.

2. Reboilers for columns, using relatively small size direct-fired units.
3. Direct-fired reactors, for example, the pyrolysis of dichloroethane to form vinyl chloride.
4. Interstage reheaters for high-temperature endothermic reactions.
5. Reformers for hydrogen production, giving outlet temperatures of 800 to 900 °C.
6. Steam boilers.
7. Heaters for hot oil circuits.

19.17.1 Basic construction

Many different designs and layouts are used, depending on the application; see Berman (1979a) and Trinks et al. (2004).

The basic construction consists of a rectangular or cylindrical steel chamber, lined with refractory bricks. Tubes are arranged around the wall in either horizontal or vertical banks. The fluid to be heated flows through the tubes. Typical layouts are shown in Fig. 19.66 (a, b, and c). A more detailed diagram of a pyrolysis furnace is given in Fig. 19.67.

Heat transfer to the tubes on the furnace walls is predominantly by radiation. In modern designs, this radiant section is surmounted by a smaller section in which the combustion gases flow over banks of tubes and transfer heat by convection. Extended surface tubes, with fins or pins, can be used in the convection section to improve the heat transfer from the combustion gases. Plain tubes known as *shock tubes* are used in the bottom rows of the convection section to act as a heat shield from the hot gases in the radiant section. Heat transfer to the shock tubes will be by both radiation and convection. The tube sizes used will normally be between 75 and 150 mm diameter. The tube size and number of passes used depend on the application and the process-fluid flow rate. Typical tube velocities are from 1 to 2 m/s for heaters, with lower rates used for reactors. Carbon steel is used for low-temperature duties; stainless steel and special alloy steels are used for elevated temperatures. For high temperatures, a material that resists creep must be used. Special metallurgies are also needed if the process fluid undergoes coking or can cause metal dusting corrosion, or if it is a mixed oxidizing-sulfiding gas that attacks the metal surface; see Chapter 6.

The burners are positioned at the base or along the sides of the radiant section. The combustion air may be pre-heated in tubes in the convection section.

The fuel is typically natural gas, fuel oil, or off-gases from the process. When process off-gases are used, they are often blended with natural gas to allow for start-up and to dampen out any variations in the fuel quality. The selection of fuel is determined by cost and environmental constraints. It will sometimes be necessary to use a more expensive fuel to meet the requirements of environmental emissions permits.

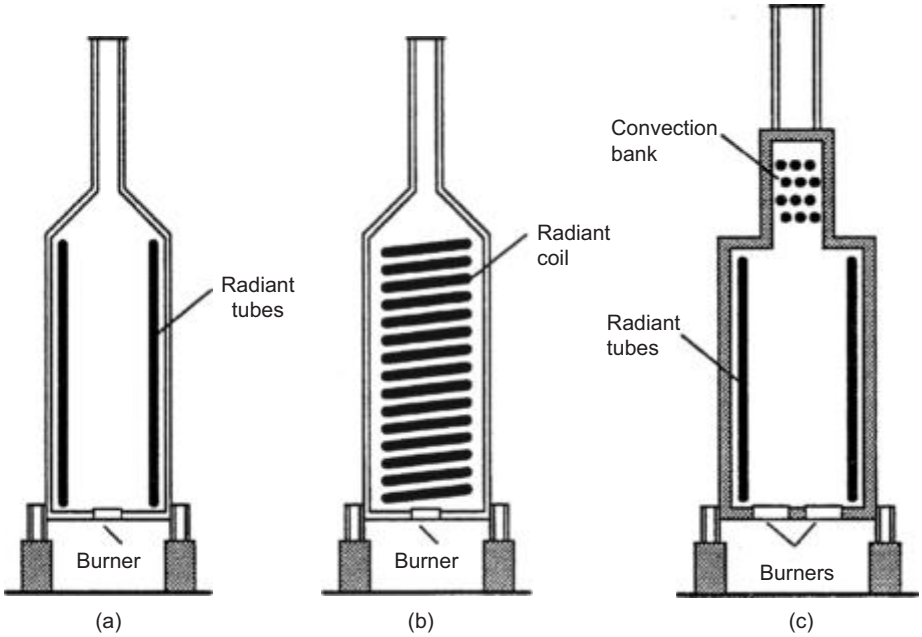


FIG. 19.66 Fired heaters. (a) Vertical-cylindrical, all radiant. (b) Vertical-cylindrical, helical coil. (c) Vertical-cylindrical with convection section.

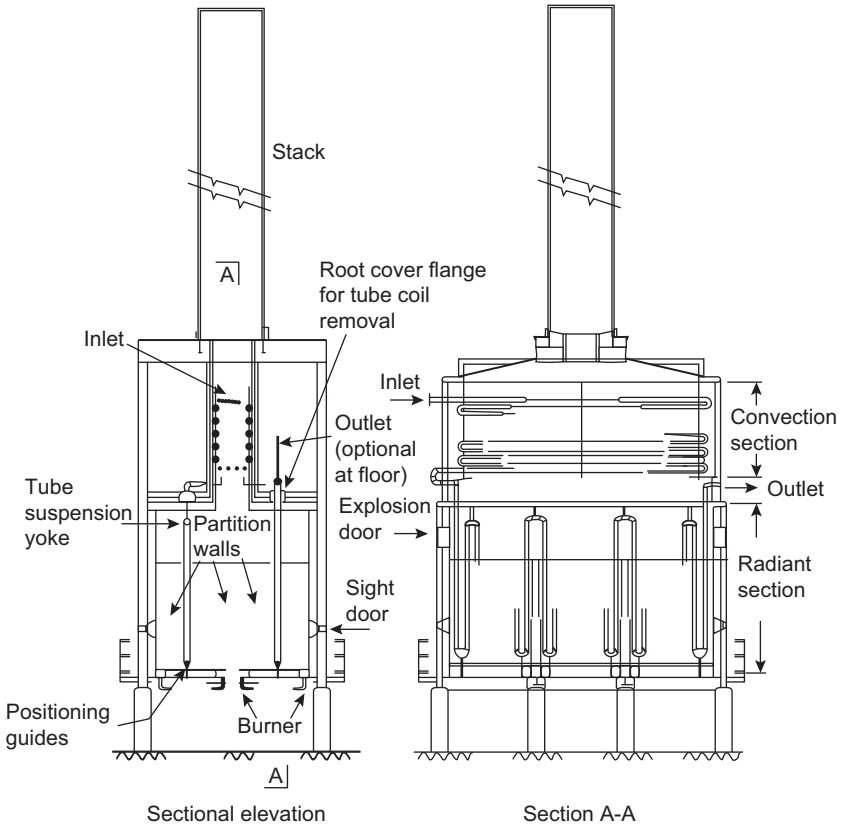


FIG. 19.67 (Foster Wheeler) Multizoned pyrolysis furnace.

19.17.2 Design of fired heaters

Commercial computer programs for the design of fired heaters are available from HTFS and HTRI; see Section 19.1. Manual calculation methods, suitable for the preliminary design of fired heaters, are given by Kern (1950), Wimpress (1978), and Evans (1980). A good overview of fired heater design and optimization is given by Zhu (2014). A brief review of the factors to be considered is given in the following sections.

19.17.3 Heat transfer in fired heaters

Radiant section

Between 50% and 70% of the total heat is transferred in the radiant section. The gas temperature depends on the fuel used and the amount of excess air. Around 20% excess air is normally used for gaseous fuels and 25% for liquid fuels. Excess air is used to prevent the formation of soot and carbon monoxide. The effect of increasing excess air is to reduce the adiabatic flame temperature and increase the stack gas flow rate, hence shifting heat availability from the radiant section to the convective section.

Radiant heat transfer from a surface is governed by the Stefan–Boltzmann equation:

$$q_r = \sigma T^4 \tag{19.66}$$

where q_r = radiant heat flux, W/m^2
σ = Stefan–Boltzmann constant, 5.67×10^{-8} W/m^2 K^4
T = temperature of the surface, K

For the exchange of heat between the combustion gases and the hot tubes, the equation can be written as:

$$Q_r = \sigma(\alpha A_{cp}) F\left(T_g^4 - T_t^4\right) \tag{19.67}$$

where Q_r = radiant heat transfer rate, W
A_{cp} = the "cold-plane" area of the tubes
= number of tubes × the exposed length × tube pitch
α = the absorption efficiency factor
F = the radiation exchange factor
T_g = temperature of the hot gases, K
T_t = tube surface temperature, K

Part of the radiation from the hot combustion gases will strike the tubes and be absorbed, and part will pass through the spaces between the tubes and be radiated back into the furnace. If the tubes are in front of the wall, some of the radiation from the wall will also be absorbed by the tubes. This complex situation is allowed for by calculating what is known as the cold plane area of the tubes, A_{cp}, and then applying the absorption efficiency factor α to allow for the fact that the tube area will not be as effective as a plane area. The absorption efficiency factor is a function of the tube arrangement and will vary from around 0.4 for widely spaced tubes to 1.0 for the theoretical situation when the tubes are touching. It will be around 0.7 to 0.8 when the pitch equals the tube diameter. Values for α are available in handbooks for different tube arrangements; see Green and Southard (2018) and Wimpress (1978).

The radiation exchange factor, F, depends on the arrangement of the surfaces and their emissivity and absorptivity. Combustion gases are poor radiators because only the carbon dioxide and water vapor, about 20% to 25% of the total, will emit radiation in the thermal spectrum. For a fired heater, the exchange factor depends on the partial pressure and emissivity of these gases and the layout of the heater. The partial pressure is dependent on the kind of fuel used, liquid or gas, and the amount of excess air. The gas emissivity is a function of temperature. Methods for estimating the exchange factor for typical furnace designs are given in the handbooks; see Green and Southard (2018) and Wimpress (1978).

The heat flux to the tubes in the radiant section will be between 20 and 40 kW/m^2 for most applications. A value of 30 kW/m^2 can be used to make a rough estimate of the tube area needed in this section.

A small amount of heat will be transferred to the tubes by convection in the radiant section, but as the superficial velocity of the gases will be low, the heat transfer coefficient will be low, around 10 W/m$^{2\circ}$C.

The temperature of the flue gas leaving the radiant section is known as the bridgewall temperature. This temperature can be estimated by assuming that roughly 60% of the heat released by combustion is transferred to the process fluid in the radiant section. The bridgewall temperature is needed for detailed design of the convective section.

Convection section

The combustion gases flow across the tube banks in the convection section, and the correlations for cross-flow in tube banks can be used to estimate the heat transfer coefficient. The gas-side coefficient will be low, and where extended surfaces are used, an allowance must be made for the fin efficiency. Procedures are given in the tube vendors' literature and in handbooks; see Section 19.14 and Berman (1978b).

The overall coefficient will depend on the gas velocity and temperature and the tube size. Typical values range from 20 to 50 W/m$^{2\circ}$C.

The shock tubes in the lower rows of the convection section receive heat by radiation from the radiant section. This can be allowed for by including the area of the lower row of tubes with the tubes in the radiant section.

19.17.4 Pressure drop

Most of the pressure drop on the flue gas side occurs in the convection section. The procedures for estimating the pressure drop across banks of tubes can be used to estimate the pressure drop in this section; see Section 19.9.3.

The pressure drop in the radiant section will be small compared with that across the convection section and can usually be neglected.

19.17.5 Process-side heat transfer and pressure drop

The tube-inside heat transfer coefficients and pressure drop can be calculated using the conventional methods for flow inside tubes; see Section 19.8. If the unit is being used as a vaporizer, the existence of two-phase flow in some of the tubes must be taken into account. Berman (1978b) gives a quick method for estimating two-phase pressure drop in the tubes of fired heaters.

Typical approach temperatures, flue gas to inlet process fluid, are around 100 °C.

19.17.6 Stack design

Most fired heaters operate with natural draft, and the stack height must be sufficient to achieve the flow of combustion air required and to remove the combustion products.

It is normal practice to operate with a slight vacuum throughout the heater so that air will leak in through sight-boxes and dampers, rather than combustion products leak out. Typically, the aim would be to maintain a vacuum of around 2 mm water gauge just below the convection section.

The stack height required depends on the temperature of the combustion gases leaving the convection section and the elevation of the site above sea level. The draft arises from the difference in density of the hot gases and the surrounding air.

The draft in millimeters of water (mm H_2O) can be estimated using the equation:

$$P_d = 0.35(L_s)(p')\left[\frac{1}{T_a} - \frac{1}{T_{ga}}\right] \tag{19.68}$$

where L_s = stack height, m
p' = atmospheric pressure, millibar ($N/m^2 \times 10^{-2}$)
T_a = ambient temperature, K
T_{ga} = average flue gas temperature, K

Because of heat losses, the temperature at the top of the stack will be around 80 °C below the inlet temperature.

The frictional pressure loss in the stack must be added to the loss in the heater when estimating the stack draft required. This can be calculated using the usual methods for pressure loss in circular conduits; see Section 19.8. The mass velocity in the stack will be around 1.5 to 2 kg/m^2. These values can be used to determine the cross-section needed.

An approximate estimate of the pressure losses in the convection section can be made by multiplying the velocity head ($u^2/2g$) by factors for each restriction; typical values are given here:

0.2 to 0.5 for each row of plain tubes
1.0 to 2.0 for each row of finned tubes
0.5 for the stack entrance
1.0 for the stack exit
1.5 for the stack damper

19.17.7 Thermal efficiency

Modern fired heaters operate at thermal efficiencies of between 80% and 90%, depending on the fuel and the excess air requirement. In some applications, additional excess air may be used to reduce the flame temperature to avoid overheating of the tubes. If only the radiant section is used, the efficiency is in the range 60% to 65%.

Where the inlet temperature of the process fluid is such that the outlet temperature from the convection section would be excessive, giving low thermal efficiency, this excess heat can be used to pre-heat the air to the furnace. Tubes would be installed above the process fluid section in the convection section. Forced-draft operation would be needed to drive the air flow through the pre-heat section.

Heat losses from the heater casing are normally between 1.5% and 2.5% of the heat input.

The largest contribution to heat losses is the sensible heat of the flue gas leaving the stack. There are several practical limits on how much heat can be recovered from the flue gas:

1. For process control reasons, the process heating duty is often carried out in the radiant section only; see Chapter 5.
2. There may not be sufficient process heat requirement in the lower temperature range of the convection section. In this case, the convection section can be used to raise steam or pre-heat boiler feed water if the heat recovered justifies the cost of the additional piping required.
3. The stack gas should not be cooled to the dew point; otherwise, condensation can occur, leading to corrosion of the stack. The presence of carbon dioxide and sulfur oxides from the combustion reactions in the flue gas raises the dew point and causes the condensate to be acidic.
4. A large temperature difference is usually specified between the flue gas and the process fluid so as to decrease the tube cost in the convection section. This leads to high stack temperatures.

5. Many companies avoid cooling the flue gas close to the dew point to prevent the formation of a visible plume from the stack. If the flue gas leaving the stack is near the dew point, then when it mixes with cold ambient air, a mist will form. This gives the stack the appearance of smoking. If the flue gas is hotter, the gas can disperse before condensation occurs and the plume is eliminated. The general public prefers not to see plumes coming from chemical plants, so public relations often triumphs over energy efficiency.

19.17.8 Fired heater emissions

Fired heaters are a major source of atmospheric emissions and are tightly regulated. Permits are usually required for operation of process heaters, and modifications to the heater or burners often require approval from environmental agencies or reissuance of the permit.

Fired heater emissions concerns include:

1. Carbon monoxide, unburned hydrocarbons, and soot can be formed if combustion is not complete. These emissions are usually minimized by operating with at least 20% excess air.
2. Sulfur oxides and metals can be emitted if sulfur or metals were present in the fuel. These emissions occur mainly when burning heavy fuel oils. Emissions of sulfur oxides can be reduced by switching to a fuel with lower sulfur content, such as natural gas.
3. Nitrogen oxides, NO_x, are formed during combustion. Unfortunately, use of excess air tends to make NO_x formation worse. Formation of NO_x is controlled by using special burner designs such as staged-air or staged-fuel burners, by using steam injection or flue gas recirculation to reduce the flame temperature, or by catalytic decomposition of the NO_x in the flue gas.
4. Carbon dioxide is formed from combustion of hydrocarbon fuels. The penalties for CO_2 emissions are not yet large enough to drive companies to recover CO_2 from flue gas, but CO_2 can be recovered by scrubbing if necessary. Carbon dioxide capture can be made easier by using novel furnace designs in which the fuel is burnt in oxygen and recirculating carbon dioxide—a system known as "oxyfuel combustion."

19.18 Heat transfer to vessels

The simplest way to transfer heat to a process or storage vessel is to fit an external jacket or an internal coil. If these methods cannot provide sufficient heat transfer area, a stream is withdrawn from the vessel, pumped through a heat exchanger, and returned to the vessel.

19.18.1 Jacketed vessels

Conventional jackets

The most commonly used type of jacket is that shown in Fig. 19.68. It consists of an outer cylinder that surrounds part of the vessel. The heating or cooling medium circulates in the annular space between the jacket and vessel walls, and the heat is transferred through the wall of the vessel. Circulation baffles are usually installed in the annular space to increase the velocity of the liquid flowing through the jacket and improve the heat transfer coefficient

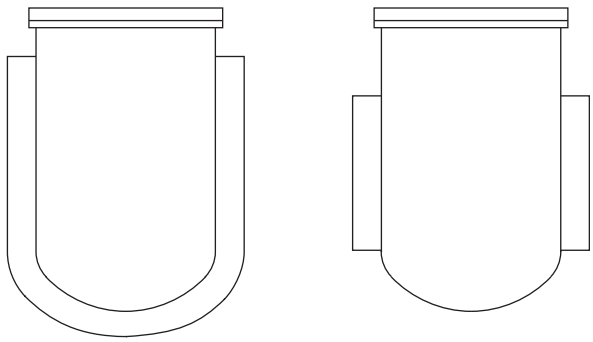


FIG. 19.68 Jacketed vessel.

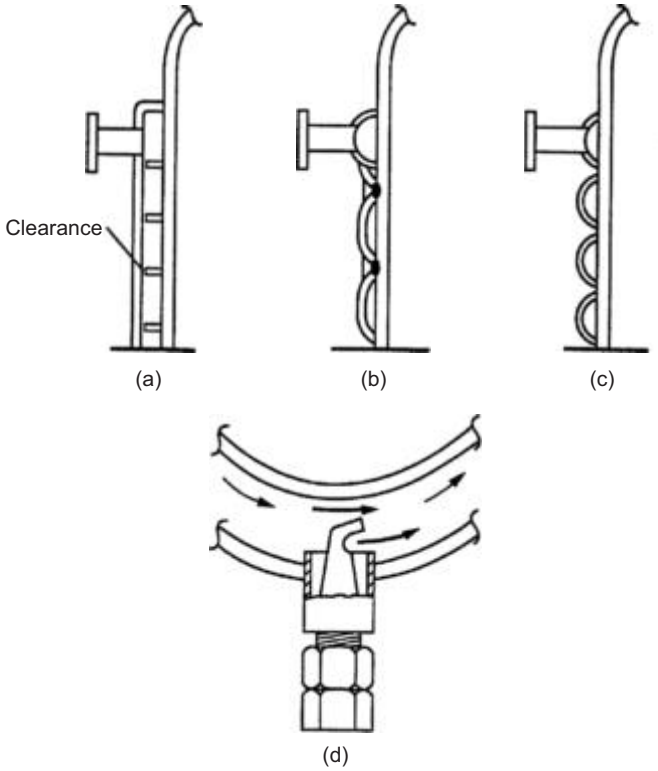


FIG. 19.69 Jacketed vessels. (a) Spirally baffled jacket. (b) Dimple jacket. (c) Half-pipe jacket. (d) Agitation nozzle.

(Fig. 19.69a). The same effect can be obtained by introducing the fluid through a series of nozzles spaced down the jacket. The momentum of the jets issuing from the nozzles sets up a swirling motion in the jacket liquid (see Fig. 19.69d). The spacing between the jacket and vessel wall will depend on the size of the vessel, but will typically range from 50 mm for small vessels to 300 mm for large vessels.

Half-pipe jackets

Half-pipe jackets are formed by welding sections of pipe, cut in half along the longitudinal axis, to the vessel wall. The pipe is usually wound around the vessel in a helix (Fig. 19.69c).

The pitch of the coils and the area covered can be selected to provide the heat transfer area required. Standard pipe sizes are used, ranging from 60 to 120 mm outside diameter. The half-pipe construction makes a strong jacket capable of withstanding pressure better than the conventional jacket design.

Dimpled jackets

Dimpled jackets are similar to the conventional jackets, but are constructed of thinner plates. The jacket is strengthened by a regular pattern of hemispherical dimples pressed into the plate and welded to the vessel wall (see Fig. 19.69b).

Jacket selection

Factors to consider when selecting the type of jacket to use are:

1. Cost: In terms of cost, the designs can be ranked, from cheapest to most expensive, as:
   simple, no baffles
   agitation nozzles
   spiral baffle
   dimple jacket
   half-pipe jacket
2. Heat transfer rate required: Select a spirally baffled or half-pipe jacket if high rates are required.
3. Pressure: As a rough guide, the pressure rating of the designs can be taken as:

jackets, up to 10 bar
dimpled jackets, up to 20 bar
half-pipe, up to 70 bar.

So, half-pipe jackets would be used for high pressure.

Jacket heat transfer and pressure drop

The heat transfer coefficient to the vessel wall can be estimated using the correlations for forced convection in conduits, such as Equation 19.11. The fluid velocity and the path length can be calculated from the geometry of the jacket arrangement. The hydraulic mean diameter (equivalent diameter, d_e) of the channel or half-pipe should be used as the characteristic dimension in the Reynolds and Nusselt numbers; see Section 19.8.1.

In dimpled jackets, a velocity of 0.6 m/s can be used to estimate the heat transfer coefficient. A method for calculating the heat transfer coefficient for dimpled jackets is given by Makovitz (1971).

The coefficients for jackets using agitation nozzles are similar to those given by using baffles. A method for calculating the heat transfer coefficient using agitation nozzles is given by Bolliger (1982).

To increase heat transfer rates, the velocity through a jacket can be increased by recirculating the cooling or heating liquid.

For simple jackets without baffles, heat transfer will be mainly by natural convection, and the heat transfer coefficient will range from 200 to 400 $W/m^{2\circ}C$.

When steam is used in a jacket, the heat transfer coefficient is in the range of 4000 to 5000 $W/m^{2\circ}C$.

19.18.2 Internal coils

The simplest and cheapest form of heat transfer surface for installation inside a vessel is a helical coil (Fig. 19.70). The pitch and diameter of the coil can be made to suit the application and the area required. The diameter of the pipe used for the coil is typically equal to $D_v/30$, where D_v is the vessel diameter. The coil pitch is usually around twice the pipe diameter. Small coils can be self-supporting, but for large coils some form of supporting structure will be necessary. Single- or multiple-turn coils are used.

Coil heat transfer and pressure drop

The heat transfer coefficient at the inside wall and pressure drop through the coil can be estimated using the correlations for flow through pipes; see Section 19.8. Correlations for forced convection in coiled pipes are also given in the ESDU Design Guide, ESDU 78031 (2001).

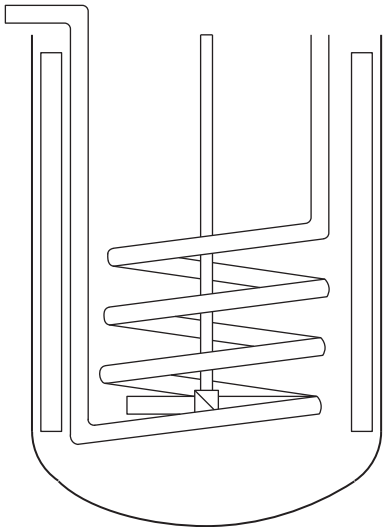


FIG. 19.70 Internal coils.

19.18.3 Agitated vessels

Unless only small rates of heat transfer are required, as when maintaining the temperature of liquids in storage vessels, some form of agitation will be needed. The various types of agitator used for mixing and blending described in Chapter 15, Section 15.5, are also used to promote heat transfer in vessels. The correlations used to estimate the heat transfer coefficient to the vessel wall, or to the surface of coils, have the same form as those used for forced convection in conduits; see Equation 19.10. The fluid velocity is replaced by a function of the agitator diameter and rotational speed, $D \times N$, and the characteristic dimension is the agitator diameter.

$$\mathrm{Nu} = C\,\mathrm{Re}^{a}\,\mathrm{Pr}^{b}\left(\frac{\mu}{\mu_w}\right)^{c} \tag{19.10}$$

For agitated vessels:

$$\frac{h_v D}{k_f} = C\left(\frac{ND^2\rho}{\mu}\right)^{a}\left(\frac{C_p\mu}{k_f}\right)^{b}\left(\frac{\mu}{\mu_w}\right)^{c} \tag{19.69}$$

where h_v = heat transfer coefficient to vessel wall or coil, W/m^2°C
D = agitator diameter, m
N = agitator, speed, rps (revolutions per second)
ρ = liquid density, kg/m^3
k_f = liquid thermal conductivity, W/m°C
C_p = liquid-specific heat capacity, J/kg°C
μ = liquid viscosity, Nm^{-2}s

The values of the constant C and the indices a, b, and c depend on the type of agitator, the use of baffles, and whether the transfer is to the vessel wall or to coils. Some typical correlations are given next.

Baffles will normally be used in most applications.

1. Flat blade paddle, baffled or unbaffled vessel, transfer to vessel wall, $Re < 4000$:

$$\mathrm{Nu} = 0.36\,\mathrm{Re}^{0.67}\,\mathrm{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.70a}$$

2. Flat blade disc turbine, baffled or unbaffled vessel, transfer to vessel wall, $Re < 400$:

$$\mathrm{Nu} = 0.54\,\mathrm{Re}^{0.67}\,\mathrm{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.70b}$$

3. Flat blade disc turbine, baffled vessel, transfer to vessel wall, $Re > 400$:

$$\mathrm{Nu} = 0.74\,\mathrm{Re}^{0.67}\,\mathrm{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.70c}$$

4. Propeller, three blades, transfer to vessel wall, Re > 5000:

$$\mathrm{Nu} = 0.64\,\mathrm{Re}^{0.67}\,\mathrm{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.70d}$$

5. Turbine, flat blades, transfer to coil, baffled, Re, 2000 to 700,000:

$$\mathrm{Nu} = 1.10\,\mathrm{Re}^{0.62}\,\mathrm{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.70e}$$

6. Paddle, flat blades, transfer to coil, baffled:

$$\mathrm{Nu} = 0.87\,\mathrm{Re}^{0.62}\,\mathrm{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14} \tag{19.70f}$$

More comprehensive design data are given by Uhl and Gray (1967), Wilkinson and Edwards (1972), Penny (1983), and Fletcher (1987).

Example 19.15

A jacketed, agitated reactor consists of a vertical cylinder 1.5 m diameter with a hemispherical base and a flat, flanged top. The jacket is fitted to the cylindrical section only and extends to a height of 1 m. The spacing between the jacket and vessel walls is 75 mm. The jacket is fitted with a spiral baffle. The pitch between the spirals is 200 mm.

The jacket is used to cool the reactor contents. The coolant used is chilled water at 10 °C; flow rate 32,500 kg/h, exit temperature 20 °C.

Estimate the heat transfer coefficient at the outside wall of the reactor and the pressure drop through the jacket.

Solution

The baffle forms a continuous spiral channel, section 75 mm × 200 mm.

$$\text{Number of spirals} = \text{height of jacket/pitch} = 1/(200\times 10^{-3}) = 5$$

$$\text{Length of channel} = 5 \times \pi \times 1.5 = 23.6 \text{ m}$$

$$\text{Cross-sectional area of channel} = (75\times 200) \times 10^{-6} = 15 \times 10^{-3}\text{m}^2$$

$$\text{Hydraulic mean diameter, } d_e = \frac{4 \times \text{cross-sectional area}}{\text{wetted perimeter}}$$

$$= \frac{4 \times (75 \times 200)}{2(75 + 200)} = 109 \text{ mm}$$

Physical properties at mean temperature of 15°C, from steam tables: $\rho = 999$ kg/m^3, $\mu = 1.136$ mNm^{-2}s, Pr = 7.99, k_f = 595×10^{-3}W/m C.

$$\text{Velocity through channel, } u = \frac{32,000}{3600} \times \frac{1}{999} \times \frac{1}{15 \times 10^{-3}} = 0.602 \text{ m/s}$$

$$\text{Re} = \frac{999 \times 0.602 \times 109 \times 10^{-3}}{1.136 \times 10^{-3}} = 57,705$$

Chilled water is not viscous, so use Equation 19.11 with $C = 0.023$ and neglect the viscosity correction term.

$$\text{Nu} = 0.023\text{Re}^{0.8}\text{Pr}^{0.33}$$

$$\frac{h_j \times 109 \times 10^{-3}}{595 \times 10^{-3}} = 0.023\,(57705)^{0.8}(7.99)^{0.33} \tag{19.11}$$

$$h_j = \underline{\underline{1606}}\,\text{W/m}^2\text{°C}$$

Use Equation 19.18 for estimating the pressure drop, taking the friction factor from Fig. 19.24. As the hydraulic mean diameter will be large compared with the roughness of the jacket surface, the relative roughness will be comparable with that for heat exchanger tubes. The relative roughness of pipes and channels and the effect on the friction factor are covered in Chapter 20.

From Fig. 19.24, for Re = 5.8×10^4, $j_f = 3.2 \times 10^{-3}$:

$$\Delta P = 8 j_f \left(\frac{L}{d_e}\right) \rho \frac{u^2}{2}$$

$$\Delta P = 8 \times 3.2 \times 10^{-3} \left(\frac{23.6}{109} \times 10^{-3}\right) 999 \times \frac{0.602^2}{2} \tag{19.18}$$

$$= \underline{\underline{1003}}\ \text{N/m}^2$$

Example 19.16

The reactor described in Example 19.15 is fitted with a flat blade disc turbine agitator 0.6 m diameter, running at 120 rpm. The vessel is baffled and is constructed of stainless steel plate 10 mm thick.

The physical properties of the reactor contents are $\rho = 850$ kg/m^3, $\mu = 80$ mNm^{-2}s, $k_f = 400 \times 10^{-3}$ W/m°C, $C_p = 2.65$ kJ/kg°C.

Estimate the heat transfer coefficient at the vessel wall and the overall coefficient in the clean condition.

Solution

Agitator speed (revs per sec) $= 1200/60 = 2$ s^{-1}

$$\text{Re} = \frac{\rho N D^2}{\mu} = \frac{850 \times 2 \times 0.6^2}{80 \times 10^{-3}} = 7650$$

$$\text{Pr} = \frac{C_p \mu}{k_f} = \frac{2.65 \times 10^3 \times 80 \times 10^{-3}}{400 \times 10^{-3}} = 530$$

For a flat blade turbine use Equation 19.70(c):

$$\text{Nu} = 0.74\,\text{Re}^{0.67}\,\text{Pr}^{0.33}\left(\frac{\mu}{\mu_w}\right)^{0.14}$$

Neglect the viscosity correction term:

$$\frac{h_v \times 0.6}{400 \times 10^{-3}} = 0.74\,(7650)^{0.67}(530)^{0.33}$$

$$h_v = 1564 \text{ W/m}^2\text{°C}$$

Taking the thermal conductivity of stainless steel as 16 W/m°C and the jacket coefficient from Example 19.15:

$$\frac{1}{U} = \frac{1}{1606} + \frac{10 \times 10^{-3}}{16} + \frac{1}{1564}$$

$$U = \underline{\underline{530}} \text{ W/m}^2\text{°C}$$

19.19 Capital cost of heat transfer equipment

The capital cost of most heat transfer devices is dominated by the cost of the tubes or plates that provide the heat transfer area. Cost correlations for heat transfer devices are therefore usually expressed as a function of the heat transfer area. Cost correlations for shell and tube, double-pipe, plate-and-frame exchangers, and kettle and thermosiphon reboilers are given in Table 7.2.

For fired heaters, the heat flux through the tubes is very high. The cost of surface area is still significant, but other costs from site fabrication, refractory installation, and burners are also important. Fired heater costs are usually better correlated against heater duty than tube wall area. Costs for fired heaters are also given in Table 7.2.

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19.21 Nomenclature

		Dimensions in MLTθ
A	Heat transfer area	$\mathbf{L}^2$
A_b	Bundle cross-sectional area of an air-cooled exchanger	$\mathbf{L}^2$
A_{cp}	Cold-plane area of tubes	$\mathbf{L}^2$
A_o	Outside area of bare tube	$\mathbf{L}^2$
A_f	Fin area in Equation 19.59	$\mathbf{L}^2$
A_f	Cross-sectional area for flow in Equation 19.56	$\mathbf{L}^2$
A_o	Outside area of bare tube	$\mathbf{L}^2$
A_p	Area of a port plate heat exchanger	$\mathbf{L}^2$
A_s	Cross-flow area between tubes	$\mathbf{L}^2$
a	Index in Equation 19.10	—
b	Index in Equation 19.10	—
C	Constant in Equation 19.10	—
C_p	Heat capacity at constant pressure	$\mathbf{L}^2\mathbf{T}^{-2}\boldsymbol{\theta}^{-1}$
C_{pg}	Heat capacity of gas	$\mathbf{L}^2\mathbf{T}^{-2}\boldsymbol{\theta}^{-1}$
C_{pL}	Heat capacity of liquid phase	$\mathbf{L}^2\mathbf{T}^{-2}\boldsymbol{\theta}^{-1}$
c	Index in Equation 19.10	—
D	Agitator diameter	$\mathbf{L}$
D_b	Bundle diameter	$\mathbf{L}$
D_s	Shell diameter	$\mathbf{L}$
D_v	Vessel diameter	$\mathbf{L}$
d	Diameter	$\mathbf{L}$
d_e	Equivalent (hydraulic mean) diameter	$\mathbf{L}$
d_i	Tube inside diameter	$\mathbf{L}$
d_{pt}	Diameter of the ports in the plates of a plate heat exchanger	$\mathbf{L}$
d_o	Tube outside diameter	$\mathbf{L}$
d_1	Outside diameter of inner of concentric tubes	$\mathbf{L}$
d_2	Inside diameter of outer of concentric tubes	$\mathbf{L}$
E	Term in Equation 19.12	—
E_f	Fin efficiency	—
F	Radiation exchange factor in Equation 19.67	—

		Dimensions in MLTθ
F	Feed molar flow rate (Example 19.11)	$\mathbf{MT}^{-1}$
F_t	Log mean temperature difference correction factor	—
f_c	Two-phase flow factor	—
f_m	Temperature correction factor for mixtures	—
f_s	Nucleate boiling suppression factor	—
G	Total mass flow rate per unit area	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$
G_p	Mass flow rate per unit cross-sectional area between plates	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$
G_s	Shell-side mass flow rate per unit area	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$
G_t	Tube-side mass flow rate per unit area	$\mathbf{ML}^{-2}\mathbf{T}^{-1}$
g	Gravitational acceleration	$\mathbf{LT}^{-2}$
H_s	Sensible heat of stream	$\mathbf{ML}^{2}\mathbf{T}^{-3}$
H_t	Total heat of stream (sensible + latent)	$\mathbf{ML}^{2}\mathbf{T}^{-3}$
h_c	Mean heat transfer coefficient in condensation	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
$(h_c)_1$	Mean condensation heat transfer coefficient for a single tube	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
$(h_c)_b$	Heat transfer coefficient for condensation on a horizontal tube bundle	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
$(h_c)_{N_r}$	Mean condensation heat transfer coefficient for a tube in a row of tubes	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
$(h_c)_v$	Heat transfer coefficient for condensation on a vertical tube	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
$(h_c)_{BK}$	Condensation coefficient from Boyko–Kruzhilin correlation	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
$(h_c)_s$	Condensation heat transfer coefficient for stratified flow in tubes	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h'_c	Local condensing film coefficient, partial condenser	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_{cb}	Convective boiling heat transfer coefficient	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_{cg}	Mean effective cooling-condensing heat transfer coefficient, partial condenser	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h'_{cg}	Local effective cooling-condensing heat transfer coefficient, partial condenser	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_{df}	Fouling coefficient based on fin area	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_f	Heat transfer coefficient based on fin area	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_{fb}	Film boiling heat transfer coefficient	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_{fc}	Forced-convection coefficient calculated assuming liquid is flowing alone (Equation 19.47)	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h'_{fc}	Forced-convection heat transfer coefficient in Equation 19.46	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_g	Mean gas film heat transfer coefficient	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h'_g	Local sensible-heat transfer coefficient, partial condenser	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_i	Film heat transfer coefficient inside a tube	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_{id}	Fouling coefficient on inside of tube	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_{nb}	Nucleate boiling heat transfer coefficient	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h'_{nb}	Nucleate boiling coefficient in Equation 19.46	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_o	Heat transfer coefficient outside a tube	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_{od}	Fouling coefficient on outside of tube	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_p	Heat transfer coefficient in a plate heat exchanger	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$

		Dimensions in MLTθ
h_s	Shell-side heat transfer coefficient	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h'_t	Inside film coefficient in Boyko−Kruzhilin correlation	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
h_v	Heat transfer coefficient to vessel wall or coil	$\mathbf{MT}^{-3}\boldsymbol{\theta}^{-1}$
J	Term in Boyko−Kruzhilin correlation, Equation 19.31	—
j_h	Heat transfer factor defined by Equation 19.14	—
j_H	Heat transfer factor defined by Equation 19.15	—
j_f	Friction factor	—
K_1	Constant in Equation 19.3, from Table 19.4	—
K_2	Constant in Equation 19.40	—
K_b	Constant in Equation 19.52	—
K_i	Phase equilibrium constant for component I	—
k_f	Thermal conductivity of fluid	$\mathbf{MLT}^{-3}\theta^{-1}$
k_L	Thermal conductivity of liquid	$\mathbf{MLT}^{-3}\theta^{-1}$
k_v	Thermal conductivity of vapor	$\mathbf{MLT}^{-3}\theta^{-1}$
k_w	Thermal conductivity of tube wall material	$\mathbf{MLT}^{-3}\theta^{-1}$
L	Tube length	**L**
L	Liquid molar flow rate in Example 19.11	$\mathbf{MT}^{-1}$
L'	Effective tube length	**L**
L_P	Path length in a plate heat exchanger	**L**
L_s	Stack height	**L**
l_B	Baffle spacing (pitch)	**L**
l_f	Fin height	**L**
m	Index in Equation 19.19	—
N	Rotational speed	$\mathbf{T}^{-1}$
N_b	Number of baffles	—
N_{bk}	Number of tubes per bank	—
N_p	Number of passes	—
N_r	Number of tubes in a vertical row	—
N_t	Number of tubes in a tube bundle	—
NTU	Number of transfer units	—
n_1	Index in Equation 19.3 from Table 19.4	—
P	Total pressure	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
P_c	Critical pressure	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
P_d	Stack draft	**L**
ΔP	Pressure drop	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
ΔP_b	Pressure drop across air-cooled exchanger bundle	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
ΔP_f	Pressure drop due to friction	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
ΔP_p	Pressure drop in a plate heat exchanger	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$
ΔP_{pt}	Pressure loss through the ports in a plate heat exchanger	$\mathbf{ML}^{-1}\mathbf{T}^{-2}$

		Dimensions in MLTθ
ΔP_s	Shell-side pressure drop	$\mathbf{ML^{-1}T^{-2}}$
ΔP_s	Static pressure in thermosiphon tubes	$\mathbf{ML^{-1}T^{-2}}$
ΔP_t	Tube-side pressure drop	$\mathbf{ML^{-1}T^{-2}}$
p'	Atmospheric pressure	$\mathbf{ML^{-1}T^{-2}}$
p_f	Fin pitch	**L**
p_s	Saturation vapor pressure	$\mathbf{ML^{-1}T^{-2}}$
p_t	Tube pitch	**L**
p_w	Saturation vapor pressure corresponding to wall temperature	$\mathbf{ML^{-1}T^{-2}}$
Q	Heat transferred in unit time	$\mathbf{ML^{2}T^{-3}}$
Q_g	Sensible heat transfer rate from gas phase	$\mathbf{ML^{2}T^{-3}}$
Q_r	Radiant heat transfer rate	$\mathbf{ML^{2}T^{-3}}$
Q_t	Total heat transfer rate from gas phase	$\mathbf{ML^{2}T^{-3}}$
q	Heat flux (heat transfer rate per unit area)	$\mathbf{MT^{-3}}$
q'	Uncorrected value of flux from Fig. 19.55	$\mathbf{MT^{-3}}$
q_c	Maximum (critical) flux for a single tube	$\mathbf{MT^{-3}}$
q_{cb}	Maximum flux for a tube bundle	$\mathbf{MT^{-3}}$
q_r	Radiant heat flux	$\mathbf{MT^{-3}}$
R	Dimensionless temperature ratio defined by Equation 19.6	—
S	Dimensionless temperature ratio defined by Equation 19.7	—
T	Shell-side temperature	**θ**
T	Temperature of surface	**θ**
T_a	Ambient temperature	**θ**
T_{bi}	Temperature of liquid entering reboiler	**θ**
T_{bo}	Temperature of vapor leaving reboiler	**θ**
T_c	Critical temperature	**θ**
T_g	Temperature of combustion gases	**θ**
T_{ga}	Average flue-gas temperature	**θ**
T_r	Reduced temperature	—
T_s	Saturation temperature	**θ**
T_{sat}	Saturation temperature	**θ**
T_t	Tube surface temperature	**θ**
T_v	Vapor (gas) temperature	**θ**
T_w	Wall (surface) temperature	**θ**
T_1	Hot-side inlet temperature	**θ**
T_2	Hot-side exit temperature	**θ**
ΔT	Temperature difference	**θ**
ΔT_{lm}	Logarithmic mean temperature difference	**θ**
ΔT_m	Mean temperature difference in Equation 19.1	**θ**
ΔT_s	Temperature change in vapor (gas) stream	**θ**

		Dimensions in MLTθ
t	Tube-side temperature	θ
t	Water temperature in Equation 19.17	θ
t_c	Local coolant temperature	θ
t_f	Fin thickness	L
t_i	Stream inlet temperature	θ
t_o	Stream outlet temperature	θ
t_w	Estimated wall temperature	θ
t_1	Cold-side inlet temperature	θ
t_2	Cold-side exit temperature	θ
U	Overall heat transfer coefficient	$\mathbf{MT^{-3}}\theta^{-1}$
U'	Uncorrected overall coefficient, Equation 19.51	$\mathbf{MT^{-3}}\theta^{-1}$
U_c	Corrected overall coefficient, Equation 19.52	$\mathbf{MT^{-3}}\theta^{-1}$
U_o	Overall heat transfer coefficient based on tube outside area	$\mathbf{MT^{-3}}\theta^{-1}$
U_1, U_2	Overall heat transfer coefficients evaluated at the ends of the exchanger	$\mathbf{MT^{-3}}\theta^{-1}$
u	Fluid velocity	$\mathbf{LT^{-1}}$
u_L	Liquid velocity, Equation 19.34	$\mathbf{LT^{-1}}$
u_p	Fluid velocity in a plate heat exchanger	$\mathbf{LT^{-1}}$
u_{pt}	Velocity through the ports of a plate heat exchanger	$\mathbf{LT^{-1}}$
u_p	Velocity through channels of a plate heat exchanger	$\mathbf{LT^{-1}}$
u_s	Shell-side fluid velocity	$\mathbf{LT^{-1}}$
u_t	Tube-side fluid velocity	$\mathbf{LT^{-1}}$
u_v	Vapor velocity, Equation 19.34	$\mathbf{LT^{-1}}$
$\hat{u}_v$	Maximum vapor velocity in kettle reboiler	$\mathbf{LT^{-1}}$
V	Vapor molar flow rate	$\mathbf{MT^{-1}}$
v_i	Specific volume at inlet	$\mathbf{L^3M^{-1}}$
v_o	Specific volume at outlet	$\mathbf{L^3M^{-1}}$
W	Mass flow rate of fluid	$\mathbf{MT^{-1}}$
W_c	Total condensate mass flow rate	$\mathbf{MT^{-1}}$
W_s	Shell-side fluid mass flow rate	$\mathbf{MT^{-1}}$
w	Mass flow through the channels and ports in a plate heat exchanger	$\mathbf{MT^{-1}}$
w_f	Fan power	$\mathbf{ML^2T^{-3}}$
X_{tt}	Lockhart–Martinelli two-phase flow parameter	—
x	Mass fraction of vapor	—
x_i	Mole fraction of component i in liquid phase	—
y_i	Mole fraction of component i in vapor phase	—
Z	Ratio of change in sensible heat to change in total heat of gas stream (sensible + latent)	—
z_i	Mole fraction of component i in feed	—
a	Absorption efficiency factor	—

		Dimensions in MLTθ
Γ	Tube loading	$\mathbf{ML^{-1}T^{-1}}$
Γ_h	Condensate loading on a horizontal tube	$\mathbf{ML^{-1}T^{-1}}$
Γ_v	Condensate loading on a vertical tube	$\mathbf{ML^{-1}T^{-1}}$
η_f	Fan efficiency	—
λ	Latent heat	$\mathbf{L^2T^{-2}}$
μ	Viscosity at bulk fluid temperature	$\mathbf{ML^{-1}T^{-1}}$
μ_L	Liquid viscosity	$\mathbf{ML^{-1}T^{-1}}$
μ_v	Vapor viscosity	$\mathbf{ML^{-1}T^{-1}}$
μ_w	Viscosity at wall temperature	$\mathbf{ML^{-1}T^{-1}}$
ρ	Fluid density	$\mathbf{ML^{-3}}$
ρ_L	Liquid density	$\mathbf{ML^{-3}}$
ρ_m	Mean density	$\mathbf{ML^{-3}}$
ρ_v	Vapor density	$\mathbf{ML^{-3}}$
σ	Stephan–Boltzmann constant in Equation 19.66	$\mathbf{MT^{-3}\theta^{-4}}$
σ	Surface tension	$\mathbf{MT^{-3}}$
Dimensionless numbers		
Nu	Nusselt number	—
Pr	Prandtl number	—
Pr_c	Prandtl number for condensate film	—
Re	Reynolds number	—
Re_c	Reynolds number for condensate film	—
Re_L	Reynolds number for liquid phase	—
St	Stanton number	—

19.22 Problems

19.1. A solution of sodium hydroxide leaves a dissolver at 80 °C and is to be cooled to 40 °C using cooling water. The maximum flow rate of the solution will be 8000 kg/h. The maximum inlet temperature of the cooling water will be 20 °C, and the temperature rise is limited to 20 °C.
Design a double-pipe exchanger for this duty, using standard carbon steel pipe and fittings. Use pipe of 50 mm inside diameter, 55 mm outside diameter for the inner pipe, and 75 mm inside diameter pipe for the outer. Make each section 5 m long. The physical properties of the caustic solution are:

Temperature, °C	**40**	**80**
specific heat, kJkg^{-1}°C^{-1}	3.84	3.85
density, kg/m^3	992.2	971.8
thermal conductivity, W/m°C	0.63	0.67
viscosity, mN m^{-2} s	1.40	0.43

19.2. A double-pipe heat exchanger is to be used to heat 6000 kg/h of 22 mol% hydrochloric acid. The exchanger will be constructed from karbate (impervious carbon) and steel tubing. The acid will flow through the inner karbate tube, and saturated steam at 100 °C will be used for heating. The tube dimensions will be

karbate tube inside diameter 50 mm, outside diameter 60 mm; steel tube inside diameter 100 mm. The exchanger will be constructed in sections, with an effective length of 3 m each.
How many sections will be needed to heat the acid from 15 °C to 65 °C?
Physical properties of 22% HCl at 40 °C: specific heat 4.93 $kJkg^{-1}{}^{\circ}C^{-1}$, thermal conductivity 0.39 W/m°C, density 866 kg/m^3.

Viscosity:	temperature	20	30	40	50	60	70 °C
	mN $m^{-2}s$	0.68	0.55	0.44	0.36	0.33	0.30

Karbate thermal conductivity 480 W/m°C.

19.3. In a food processing plant there is a requirement to heat 50,000 kg/h of town water from 10 °C to 70 °C. Steam at 2.7 bar is available for heating the water. An existing heat exchanger is available, with the following specifications:

Shell inside diameter 337 mm, E type
Baffles 25% cut, set at a spacing of 106 mm
Tubes 15 mm inside diameter, 19 mm outside diameter, 4094 mm long
Tube pitch 24 mm, triangular
Number of tubes 124, arranged in a single pass
Would this exchanger be suitable for the specified duty?

19.4. Design a shell and tube exchanger to heat 50,000 kg/h of liquid ethanol from 20 °C to 80 °C. Steam at 1.5 bar is available for heating. Assign the ethanol to the tube side. The total pressure drop must not exceed 0.7 bar for the alcohol stream. Plant practice requires the use of carbon steel tubes, 25 mm inside diameter, 29 mm outside diameter, 4 m long.
Set out your design on a data sheet and make a rough sketch of the heat exchanger. The physical properties of ethanol can be readily found in the literature.

19.5. 4500 kg/h of ammonia vapor at 6.7 bara pressure is to be cooled from 120 °C to 40 °C using cooling water. The maximum supply temperature of the cooling water available is 30 °C, and the outlet temperature is to be restricted to 40 °C. The pressure drops over the exchanger must not exceed 0.5 bar for the ammonia stream and 1.5 bar for the cooling water.
A contractor has proposed using a shell and tube exchanger with the following specifications for this duty:

Shell: E-type, inside diameter 590 mm
Baffles: 25% cut, 300 mm spacing
Tubes: carbon steel, 15 mm inside diameter, 19 mm outside diameter, 2400 mm long, number 360
Tube arrangement: 8 passes, triangular tube pitch, pitch 23.75 mm
Nozzles: shell 150 mm inside diameter, tube headers 75 mm inside diameter
It is proposed to put the cooling water though the tubes.
Is the proposed design suitable for the duty?
Physical properties of ammonia at the mean temperature of 80 °C: specific heat 2.418 $kJkg^{-1}{}^{\circ}C^{-1}$, thermal conductivity 0.0317 W/m°C, density 4.03 kg/m^3, viscosity 1.21×10^{-5} N $m^{-2}s$.

19.6. A vaporizer is required to evaporate 10,000 kg/h of a process fluid at 6 bar. The liquid is fed to the vaporizer at 20 °C.
The plant has a spare kettle reboiler available with the following specifications:

U-tube bundle, 50 tubes, mean length 4.8 m, end to end
Carbon steel tubes, inside diameter 25 mm, outside diameter 30 mm, square pitch 45 mm
Steam at 1.7 bara will be used for heating
Check if this reboiler would be suitable for the duty specified. Only check the thermal design. You may take it that the shell will handle the vapor rate.
Take the physical properties of the process fluid as liquid: density 535 kg/m^3, specific heat 2.6 $kJ.kg^{-1}{}^{\circ}C^{-1}$, thermal conductivity 0.094 W/m°C, viscosity 0.12 mN $m^{-2}s$, surface tension 0.85 N/m, heat of vaporization 322 kJ/kg.
Vapor density 14.4 kg/m^3.

Vapor pressure:

temperature°C	50	60	70	80	90	100	110	120
pressure bar	5.0	6.4	8.1	10.1	12.5	15.3	18.5	20.1

19.7. A condenser is required to condense n-propanol vapor leaving the top of a distillation column. The n-propanol is essentially pure and is a saturated vapor at a pressure of 2.1 bara. The condensate needs to be subcooled to 45 °C.
Design a horizontal shell and tube condenser capable of handling a vapor rate of 30,000 kg/h. Cooling water is available at 30 °C, and the temperature rise is to be limited to 30 °C. The pressure drop on the vapor stream is to be less than 50 kN/m^2 and on the water stream less than 70 kN/m^2. The preferred tube size is 16 mm inside diameter, 19 mm outside diameter, and 2.5 m long.
Take the saturation temperature of n-propanol at 2.1 bar as 118 °C. The other physical properties required can be found in the literature or estimated.

19.8. Design a vertical shell and tube condenser for the duty given in Question 19.7. Use the same preferred tube size.

19.9. In the manufacture of methyl ethyl ketone (MEK) from 2-butanol, the reactor products are precooled and then partially condensed in a shell and tube exchanger. A typical analysis of the stream entering the condenser is mol fractions: MEK 0.47, unreacted alcohol 0.06, hydrogen 0.47. Only 85% of the MEK and alcohol are condensed. The hydrogen is noncondensable.
The vapors enter the condenser at 125 °C and the condensate and uncondensed material leave at 27 °C. The condenser pressure is maintained at 1.1 bara. Make a preliminary design of this condenser for a feed rate of 1500 kg/h. Chilled water will be used as the coolant at an inlet temperature of 10 °C and allowable temperature rise of 30 °C.
Any of the physical properties of the components not available in Appendix C or the general literature should be estimated. Appendix C is available in the online material at www.elsevier.com/books-and-journals/book-companion/9780128211793.

19.10. A vertical thermosiphon reboiler is required for a column. The liquid at the base of the column is essentially pure n-butane. A vapor rate of 5 kg/s is required.
The pressure at the base of the column is 20.9 bar. Saturated steam at 5 bar will be used for heating. Estimate the number of 25 mm outside diameter, 22 mm inside diameter, 4 m long tubes needed.
At 20.9 bar the saturation temperature of n-butane is 117 °C and the heat of vaporization is 828 kJ/kg.

19.11. An immersed bundle vaporizer is to be used to supply chlorine vapor to a chlorination reactor at a rate of 10,000 kg/h. The chlorine vapor is required at 5 bar pressure. The minimum temperature of the chlorine feed will be 10 °C. Hot water at 50 °C is available for heating. The pressure drop on the water side must not exceed 0.8 bar.
Design a vaporizer for this duty. Use stainless steel U-tubes 6 m long, 21 mm inside diameter, 25 mm outside diameter, on a square pitch of 40 mm.
The physical properties of chlorine at 5 bar are saturation temperature 10 °C, heat of vaporization 260 kJ/kg, specific heat 0.99 kJkg^{-1}°C^{-1}, thermal conductivity 0.13 W/m°C, density 1440 kg/m^3, viscosity 0.3 mN m^{-2}s, surface tension 0.013 N/m, vapor density 16.3 kg/m^3.
The vapor pressure can be estimated from the equation:

$$\mathrm{Ln(P)} = 9.34 - 1978/(T + 246);\ P\ \mathrm{bar}, T^{\circ}\mathrm{C}$$

19.12. There is a requirement to cool 200,000 kg/h of a dilute solution of potassium carbonate from 70 °C to 30 °C. Cooling water will be used for cooling, with inlet and outlet temperatures of 20 °C and 60 °C.
A gasketed-plate heat exchanger is available with the following specifications:

Number of plates 329
Effective plate dimensions: length 1.5 m, width 0.5 m, thickness 0.75 mm
Channel width 3 mm
Flow arrangement two pass: two pass
Port diameters 150 mm

Check if this exchanger is likely to be suitable for the thermal duty required, and estimate the pressure drop for each stream.
Take the physical properties of the dilute potassium carbonate solution to be the same as those for water.

19.13. Design an air cooler to cool 30,000 kg/h of diesel oil from 120 °C to 50 °C. The highest ambient temperature that is exceeded for 40 h/yr on average is 40 °C.
Physical properties of diesel oil over the temperature range of interest can be taken as specific heat capacity 2.1 kJ/kg°C, thermal conductivity 0.135 W/m°C, density 800 kg/m^3, viscosity 1.2 mN m^{-2}s.

19.14. The heat duty of the jacketed vessel of Examples 19.15 and 19.16 can be estimated from the coolant flow rate and temperatures. What is the minimum temperature at which the reactor can operate using the jacket as designed? Does the choice of coolant make sense at this temperature? Propose a better design.

19.15. A stirred tank fermentation reactor has height 2 m and diameter 1.5 m and is filled with a fermentation broth that can be assumed to have the physical properties of water. The fermenter must be maintained at a temperature less than 42 °C to prevent damage to the cell culture. After allowing for sensible heat losses to the cold feed, the heat that must be removed from the fermenter is 80 kW. Cooling water is available at 20 °C and can be returned at any temperature up to 35 °C. Recommend a design for cooling the contents of the fermenter.

CHAPTER

20

Transport and storage of fluids

KEY LEARNING OBJECTIVES

- How to store gases and liquids
- How to calculate line pressure drop
- How valves, controllers, compressors, and pumps work
- How to select pumps and compressors and size piping systems and control valves

20.1 Introduction

This chapter describes the methods used for storing and transporting fluids within a process. Methods for storing and conveying solids are discussed in Chapter 18.

The design of piping systems and rotating equipment such as pumps and compressors is usually done by specialist design groups, and a detailed discussion of piping design and plant hydraulics is beyond the scope of this book. Only general guide rules are given. The piping handbook edited by Nayyar (2000) is particularly recommended for guidance on the detailed design of piping systems. The references cited in the text and listed at the end of the chapter should also be consulted.

Piping and instrumentation diagrams (P&IDs) are introduced in Chapter 5. A P&ID usually contains information on pipe sizes and ancillary valves and instruments, as well as the main process control valves. The sizing and selection of control valves must be carried out in concert with pipe sizing and pump or compressor design and selection. Accurate design of control valves requires a good understanding of process hydraulics and equipment pressure drop and so is best carried out after the major plant items have been specified.

20.2 Storage of fluids

All processes require storage of some inventory of feeds, products, solvents, or intermediate compounds. Inventories are maintained to ensure continuity of supply of feeds and products, to smooth out process operations, to allow scheduling of shipments, and to ensure the availability of solvents and consumables that may be needed by the process. Even plants that operate without local inventory usually require maintenance of inventory elsewhere in the supply chain. For example, gas processing plants often have no local inventory but rely on storage facilities located at various points in the gas distribution pipeline system. This section discusses methods used to store gases and liquids.

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20.2.1 Storage of gases

Gases can be stored at low pressure in gas holders similar to those used for town gas. The liquid-sealed type is most commonly used. These consist of a number of telescopic sections (lifts) that rise and fall as gas is added to or withdrawn from the holder. The dry-sealed type is used where the gas must be kept dry. In this type, the gas is contained by a piston moving in a large vertical cylindrical vessel. Water seal holders are intrinsically safer for use with flammable gases than the dry seal type, as any leakage through the piston seal may form an explosive mixture in the closed space between the piston and the vessel roof. Details of the construction of gas holders can be found in textbooks on gas engineering, such as Meade (1921) and Smith (1945).

Gases are stored at high pressures where this is a process requirement and to reduce the storage volume. For some gases, the volume can be further reduced by liquefying the gas by pressure or refrigeration. Cylindrical and spherical vessels (Horton spheres) are used. High-pressure gas storage vessels are designed as pressure vessels, as discussed in Chapter 14.

When a process consumes gas at a low flow rate, road or rail tankers are sometimes used to store the gas before transfer to a small process storage vessel.

Underground storage in depleted oil or gas reservoirs is used to store large quantities of natural gas to meet seasonal variations in demand. Underground storage tanks are sometimes used to maintain local inventories of natural gas for retail supply.

Industrial gases such as oxygen, nitrogen, and hydrogen that are consumed in large quantities are usually supplied to chemical plants by pipeline and are not stored on-site. The industrial gas companies contract to supply these gases "across the fence" and maintain sufficient storage and production capacity at their own facilities to ensure continuity of supply. When a chemical plant is located far from existing pipelines, the industrial gas companies will sometimes build a local plant to supply these gases.

20.2.2 Storage of liquids

Liquids are usually stored in bulk in vertical cylindrical steel tanks. Fixed- and floating-roof tanks are used. In a floating-roof tank a movable piston floats on the surface of the liquid and is sealed at the tank walls. Floating-roof tanks are used to eliminate evaporation losses and, for flammable liquids, to obviate the use of inert gas blanketing to prevent an explosive mixture forming above the liquid, as would be the situation with a fixed-roof tank.

Horizontal cylindrical tanks and rectangular tanks are also used for storing liquids, usually for relatively small quantities such as surge tanks for process intermediates.

Gas blanketing is used for fixed-roof tanks and for pressure vessels that are used to store liquids. The use of a gas bubble in the top of the vessel allows measurement of the level in the tank and prevents hydrostatic overpressure or discharge of liquid through vapor vents. Nitrogen is most commonly used for gas-blanketed storage, but natural gas, hydrogen, or fuel gas can be used if the designer does not want inert nitrogen to enter the process. Liquids that are not volatile, hazardous, or flammable can be stored in tanks that are vented to atmosphere, but care must be taken that dissolved oxygen does not introduce problems in downstream processing.

The mechanical design of fixed-roof, vertical tanks is discussed in Chapter 14, Section 14.15.

Liquid storage tanks are usually grouped together in a "tank farm" located away from the main plant area. The tank farm should preferably be downwind of the plant area so that in the event of a tank failure or leakage, flammable vapors will not be carried towards ignition sources in the plant. The tank farm must have good access to road, rail, or port facilities, depending on the method used to ship feeds and products.

Raw water can be stored in retaining ponds or underground aquifers when seasonal variations create a need for water storage. Treated water (demineralized water, deionized water, boiler feed water, distilled water, and reverse osmosis water) is usually stored in tanks to prevent recontamination. Cooling tower water is not typically stored, as the cooling water system provides an adequate inventory during operation and the system can be flushed to wastewater treatment during major maintenance.

20.3 Transport of gases and liquids

20.3.1 Gases

The type of equipment best suited for the pumping of gases in pipelines depends on the flow rate, the differential pressure required, and the operating pressure.

Reciprocating, centrifugal, and axial flow compressors are the principal types used in the chemical process industries, and the range of application of each type is shown in Fig. 20.1, which has been adapted from a similar diagram by Dimoplon (1978). A more comprehensive selection guide is given in Table 20.1. In general, fans are used where the pressure drop is small, less than 35 cm H_2O (0.03 bar); axial flow compressors for high flow rates and moderate differential pressures; centrifugal compressors for high flow rates; and, by staging, high differential pressures. Reciprocating compressors can be used over a wide range of pressures and capacities, but are normally only specified in preference to centrifugal compressors where high pressures are required at relatively low flow rates. Diagrammatic sketches of the compressors listed are given in Fig. 20.2. Gas compression is discussed in more detail in Section 20.6.

Vacuum production

The production of vacuum (subatmospheric pressure) is required for many chemical engineering processes, for example, vacuum distillation, drying, and filtration. The type of vacuum pump needed will depend on the degree of vacuum required, the capacity of the system, and the rate of air in-leakage.

Reciprocating and rotary positive displacement pumps are commonly used where moderately low vacuum is required, about 10 mmHg (0.013 bar), at moderate to high flow rates, such as in vacuum filtration.

Steam-jet ejectors are versatile and economic vacuum pumps and are frequently used, particularly in vacuum distillation. They can handle high vapor flow rates and, by using several ejectors in series, can produce low pressures, down to about 0.1 mmHg (0.13 mbar).

The operating principle of steam-jet ejectors is explained in Chhabra and Shankar (2017). Their specification, sizing, and operation are covered in a comprehensive series of papers by Power (1964). Diffusion pumps are used where very low pressures are required (hard vacuum) for processes such as molecular distillation.

For general references on the design and application of vacuum systems, see Ryan and Roper (1986) or Jousten and Nakhosteen (2016).

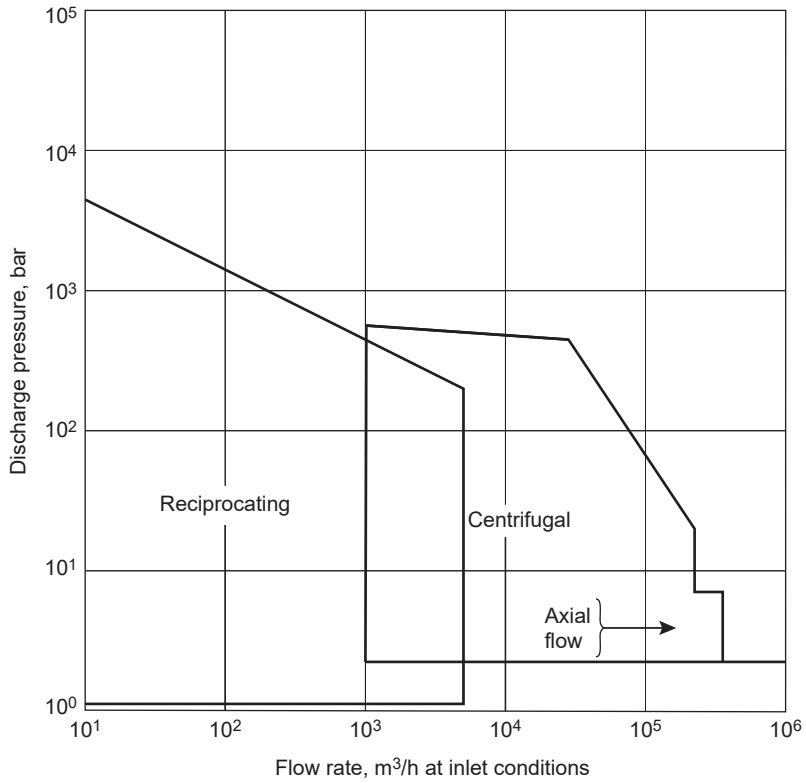


FIG. 20.1 Compressor operating ranges.

TABLE 20.1 Operating range of compressors and blowers

Type of compressor	Normal Maximum Speed (rpm)	Normal Maximum Capacity (m^3/h)	Normal Maximum Pressure (Differential) (bar)	
			Single stage	Multiple stage
Displacement				
1. Reciprocating	300	85,000	3.5	5000
2. Sliding vane	300	3400	3.5	8
3. Liquid ring	200	2550	0.7	1.7
4. Rootes	250	4250	0.35	1.7
5. Screw	10,000	12,750	3.5	17
Dynamic				
6. Centrifugal fan	1000	170,000		0.2
7. Turbo blower	3000	8500	0.35	1.7
8. Turbo compressor	10,000	136,000	3.5	100
9. Axial flow fan	1000	170,000	0.35	2.0
10. Axial flow blower	3000	170,000	3.5	10

From Begg 1966.

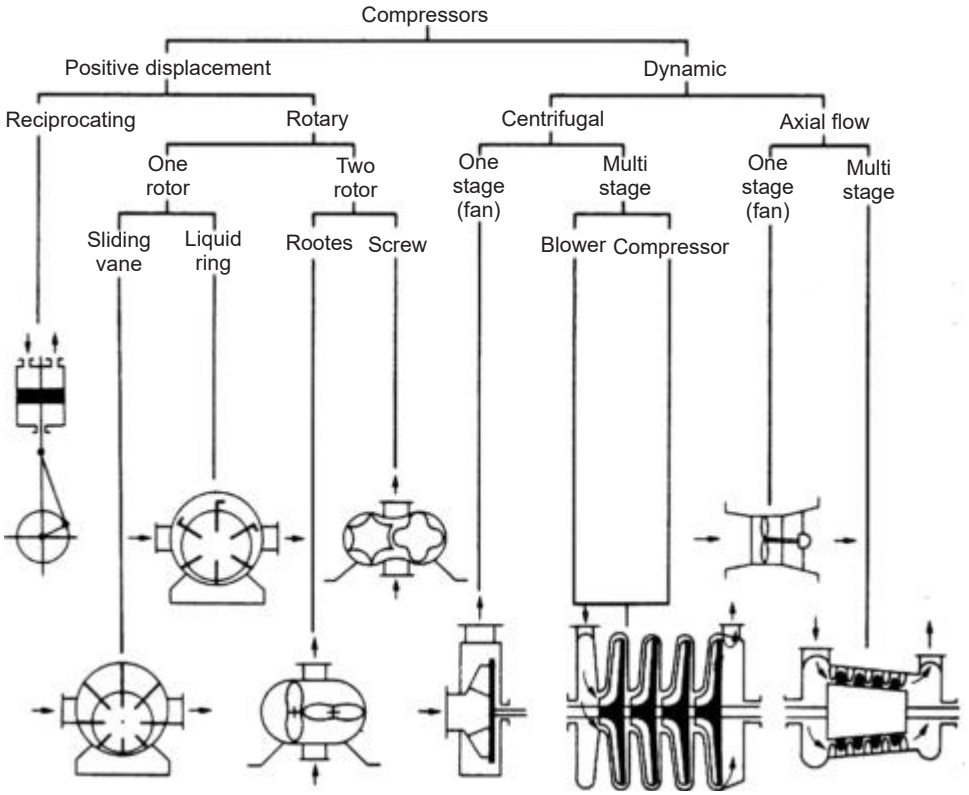


FIG. 20.2 Type of compressor. *From Begg, 1966.*

20.3.2 Liquids

Liquids and dilute slurries are almost always pumped through pipe systems. Pumps can be classified into two general types:

1. Dynamic pumps, such as centrifugal pumps
2. Positive displacement pumps, such as reciprocating and diaphragm pumps

The single-stage, horizontal, overhung centrifugal pump is by far the most common type in the chemical process industries. Other types are used where a high head or other special process considerations are specified. For example, positive displacement metering pumps are often used when small flow rates of additives must be fed to a process. Positive displacement pumps are also intrinsically easier to use with variable-speed drivers when power consumption efficiency is important; see Hall (2010). Descriptions of the types of pumps used in the chemical process industries are given in textbooks and handbooks on this subject: Garay (1997), Karassik et al. (2007), and Parmley (2000). A general guide to the selection, installation, and operation of pumps for the process industries is given by Davidson and von Bertele (2005) and Jandiel (2000).

Pump selection is made on the flow rate and head required, together with other process considerations, such as corrosion or the presence of solids in the fluid. The principal types used and their operating pressures and capacity ranges are summarized in Table 20.2. The chart shown in Fig. 20.3 can be used to determine the type of pump required for a particular head and flow rate. This figure is based on one published by Doolin (1977). For a detailed discussion of the factors governing the selection of the best centrifugal pump for a given duty, the reader should refer to the articles by De Santis (1976), Neerkin (1974), Jacobs (1965), and Couper et al. (2012). Special factors to consider when selecting a pump for slurry service are described by Nwaokocha (2019). The design and selection of centrifugal pumps are discussed in more detail in Section 20.7 and in the article by Kelly (2010).

Fig. 20.4 shows operating ranges for different types of positive displacement pumps. Centrifugal pumps will normally be the first choice for pumping process fluids, with the other types only being used for special applications, such as the use of reciprocating and gear pumps for metering. Positive displacement pumps are normally used where a high head is required at a low flow rate. Positive displacement pumps are also used for pumping highly viscous fluids. Holland and Chapman (1966) review the various types of positive displacement pumps available and discuss their applications. Hall (2010) discusses the use of positive displacement pumps with variable-speed drivers.

TABLE 20.2 Normal operating range of pumps

Type	Capacity range (m^3/h)	Typical head (m of water)
Centrifugal	0.25–103	10–50 300 (multistage)
Reciprocating	0.5–500	50–200
Diaphragm	0.05–50	5–60
Rotary gear and similar	0.05–500	60–200
Rotary sliding vane or similar	0.25–500	7–70

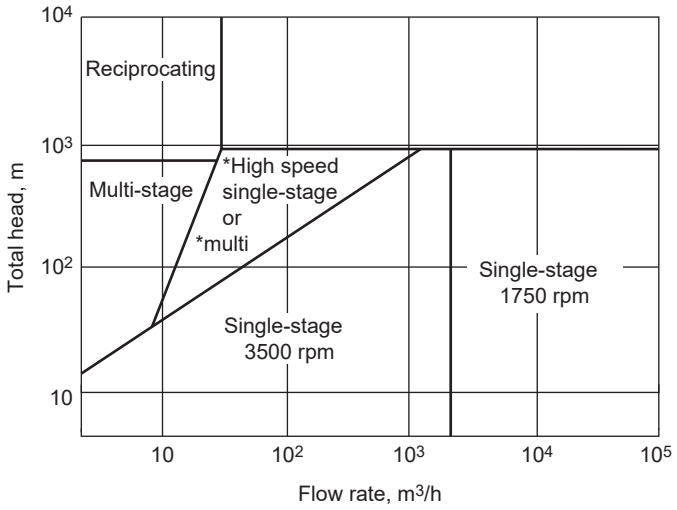


FIG. 20.3 Centrifugal pump selection guide. *Single-stage >1750 rpm, multistage 1750 rpm.

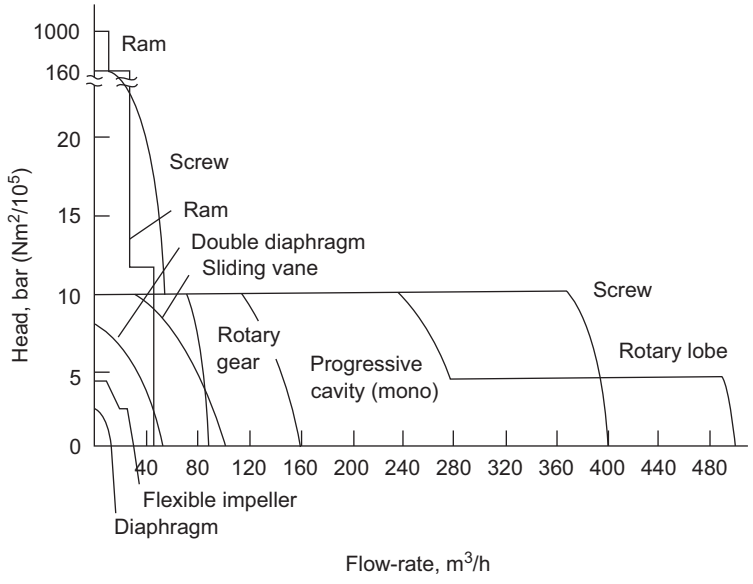


FIG. 20.4 Selection of positive displacement pumps. *Adapted from Marshall, 1985.*

20.4 Pressure drop in pipelines

Pumps, compressors, and control valves cannot be designed independently of the piping system that connects them. The pressure head that the pump or compressor must deliver is determined by the pressure drop in the process equipment and piping, the change in elevation, and the pressure drop that is required for satisfactory operation of the control valve.

20.4.1 Pressure drop in pipes

The pressure drop in a pipe due to friction is a function of the fluid flow rate, fluid density and viscosity, pipe diameter, pipe surface roughness, and length of the pipe. It can be calculated using the following equation:

$$\Delta P_f = 8f(L/d_i)\frac{\rho u^2}{2} \tag{20.1}$$

where ΔP_f = pressure drop, N/m^2

f = friction factor
L = pipe length, m
d_i = pipe inside diameter, m
ρ = fluid density, kg/m^3
u = fluid velocity, m/s

The friction factor is dependent on the Reynolds number and pipe roughness. The friction factor for use in Equation 20.1 can be found from Fig. 20.5.

$$\text{The Reynolds number is given by: } Re = (\rho \times u \times d_i)/\mu \tag{20.2}$$

where μ is the fluid viscosity. Values for the absolute surface roughness of commonly used pipes are given in Table 20.3. The parameter to use with Fig. 20.5 is the relative roughness, given by:

$$\text{relative roughness, } e = \text{absolute roughness/pipe inside diameter}$$

Note: The friction factor used in Equation 20.1 is related to the shear stress at the pipe wall, R, by the equation $f = (R/\rho\, u^2)$. Other workers use different relationships. Their charts for friction factor will give values that are multiples of those given by Fig. 20.5, so it is important to make sure that the pressure drop equation used matches the friction factor chart. One of the most commonly used is that of Fanning, which defines the coefficient of friction as $C_f = (2R/\rho\, u^2)$, that is, $C_f = 2f$, in which case Equation 20.1 becomes:

$$\Delta P_f = 4\, C_f\, (L/d_i)\, \frac{\rho u^2}{2} \tag{20.1b}$$

Non-Newtonian fluids

In Equation 20.1, and when calculating the Reynolds number for use with Fig. 20.5, the fluid viscosity and density are taken to be constant. This will be true for Newtonian liquids but not for non-Newtonian liquids, where the apparent viscosity is a function of the shear stress.

More complex methods are needed to determine the pressure drop of non-Newtonian fluids in pipelines. Suitable methods are given in Chhabra and Gurappa (2019) and in Chhabra and Richardson (2008); see also Darby (2001).

Gases

When a gas flows through a pipe, the gas density is a function of the pressure and so is determined by the pressure drop. If the pressure of the gas does not change by more than about 20%, the gas can be treated as an incompressible fluid with density equal to the density at the mean pressure. Equation 20.1 and Fig. 20.5 can then be used to estimate the pressure drop, but it may be necessary to divide the pipeline into short sections and sum the results.

For longer pipelines or low-pressure systems, the gas flow must be treated as flow of a compressible fluid. Because the density of a compressible fluid is a function of both temperature and pressure, the analysis of pipe flow becomes much more complex and sophisticated models are needed. Furthermore, it can be shown that if the pressure ratio across a restriction, valve, or pipe opening reaches a critical value, a maximum flow rate is obtained, corresponding to sonic flow at the restriction. When sonic flow occurs, further decreases in downstream pressure have no effect on the flow rate. The critical pressure ratio for an ideal gas under isothermal conditions is only 0.607, so sonic flow can easily occur. Compressible flow is discussed in Chhabra and Shankar (2017) and Teng et al. (2014).

Two-phase mixtures

For vapor–liquid mixtures, the pressure drop in horizontal pipes can be found using the correlation of Lockhart and Martinelli (1949), which relates the two-phase pressure drop to the pressure drop that would be calculated if each phase were flowing separately in the pipe. Details of the correlation and methods for two-phase flow in vertical pipes are given in Green and Southard (2018) and Chhabra and Shankar (2017).

Liquid–solid mixtures that do not settle out rapidly are usually treated as non-Newtonian fluids. This will usually be the case if the solid particle size is less than about 200 microns (0.2 mm). Larger particle sizes form settling

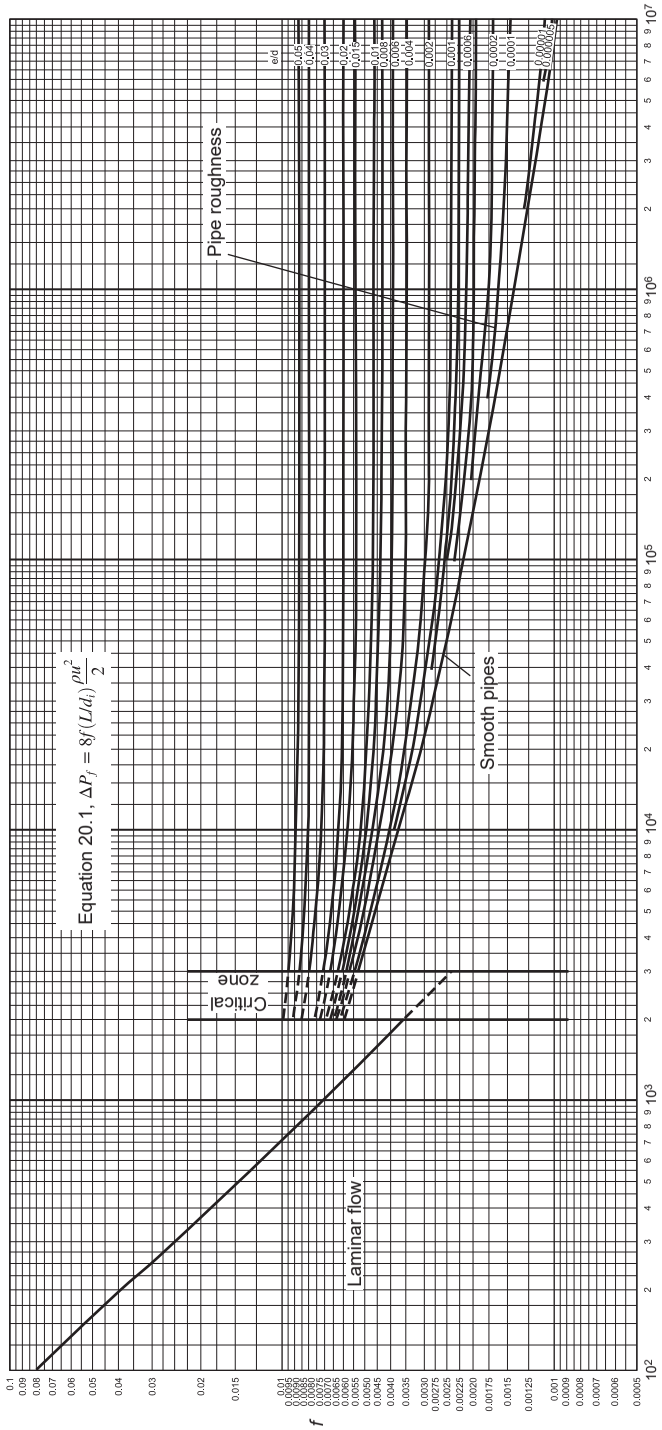


FIG. 20.5 Pipe friction versus Reynolds number and relative roughness.

TABLE 20.3 Pipe roughness

Material	Absolute roughness, mm
Drawn tubing	0.0015
Commercial steel pipe	0.046
Cast iron pipe	0.26
Concrete pipe	0.3–3.0

slurries and require a critical velocity to maintain the solids in suspension. Correlations for critical velocity and pressure drop are given in Green and Southard (2018) and Chhabra and Shankar (2017).

Gas–solid mixtures are commonly encountered in pneumatic conveying. This is discussed in Chhabra and Shankar (2017) and by Mills (2015) and Mills et al. (2004).

20.4.2 Pressure drop in pipe fittings

Any obstruction to flow will generate turbulence and cause a pressure drop, so pipe fittings such as bends, elbows, reducing or enlargement sections, and tee junctions will increase the pressure drop in a pipeline. There will also be a pressure drop due to the valves used to isolate equipment and control the fluid flow, and there can be pressure losses due to flow measurement equipment; see Livelli (2013). The pressure drop due to these miscellaneous losses can be estimated using either of two methods:

1. As the number of velocity heads, K, lost at each fitting or valve. A velocity head is $u^2/2g$, meters of the fluid, equivalent to $(\rho u^2/2)$, N/m^2, where the fluid velocity, u, is calculated at the pipe diameter. The total number of velocity heads lost due to all the fittings and valves is added to the pressure drop due to pipe friction.
2. As a length of pipe that would cause the same pressure loss as the fitting or valve. Because this will be a function of the pipe diameter, it is expressed as the number of equivalent pipe diameters. The length of pipe to add to the actual pipe length is found by multiplying the total number of equivalent pipe diameters by the diameter of the pipe being used.

The number of velocity heads lost, or equivalent pipe diameter, is a characteristic of the particular fitting or type of valve used. Values can be found in handbooks and manufacturers' literature. The values for a selected number of fittings and valves are given in Table 20.4.

The two methods used to estimate the miscellaneous losses are illustrated in Example 20.1.

Pipe fittings are discussed in Section 20.9.4; see also Green and Southard (2018). Valve types and applications are discussed in Section 20.5.

Example 20.1

A pipeline connecting two tanks contains four standard elbows, a globe valve that is fully open, and a gate valve that is half-open. The line is commercial steel pipe, 25 mm internal diameter, length 120 m.

The properties of the fluid are viscosity 0.99 mNm^{-2} s and density 998 kg/m^3. Calculate the total pressure drop due to friction when the flow rate is 3500 kg/h.

Solution

$$\text{Cross-sectional area of pipe} = \frac{\pi}{4}(25 \times 10^{-3})^2 = 0.491 \times 10^{-3} m^2$$

$$\text{Fluid velocity, } u = \frac{3500}{3600} \times \frac{1}{0.491 \times 10^{-3}} \times \frac{1}{998} = 1.98 \text{ m/s}$$

$$\text{Reynolds number, } Re = \left(998 \times 1.98 \times 25 \times 10^{-3}\right)/0.99 \times 10^{-3}$$

$$= 49,900 = 5 \times 10^4 \tag{20.2}$$

Absolute roughness commercial steel pipe, Table 20.3 = 0.046 mm

TABLE 20.4 Pressure loss in pipe fittings and valves (for turbulent flow)

Fitting or valve	*K*, number of velocity heads	number of equivalent pipe diameters
45-degree standard elbow	0.35	15
45-degree long radius elbow	0.2	10
90-degree standard radius elbow	0.6–0.8	30–40
90-degree standard long elbow	0.45	23
90-degree square elbow	1.5	75
Tee entry from leg	1.2	60
Tee entry into leg	1.8	90
Union and coupling	0.04	2
Sharp reduction (tank outlet)	0.5	25
Sudden expansion (tank inlet)	1.0	50
Gate valve		
fully open	0.15	7.5
quarter open	16	800
half open	4	200
three-fourths open	1	40
Globe valve, bevel seat-		
fully open	6	300
half open	8.5	450
Globe valve, plug-disk		
fully open	9	450
half open	36	1800
quarter open	112	5600
Plug valve – open	0.4	18

Relative roughness $= 0.046/(25 \times 10^{-3}) = 0.0018$, round to 0.002
From friction factor chart, Fig. 20.5, $f = 0.0032$

Miscellaneous losses

Fitting/valve	Number of velocity heads, *K*	Equivalent pipe diameters
Entry	0.5	25
Elbows	(0.8×4)	(40×4)
Globe valve, open	6.0	300
Gate valve, half-open	4.0	200
Exit	1.0	50
Total	14.7	735

Method 1: Velocity heads

$$\text{A velocity head} = u^2/2g = 1.98^2/(2 \times 9.8) = 0.20 \text{ m of liquid.}$$

$$\text{Head loss} = 0.20 \times 14.7 = 2.94 \text{ m}$$

$$\text{as pressure} = 2.94 \times 998 \times 9.8 = 28,754 \text{ N/m}^2$$

$$\text{Friction loss in pipe, } \Delta P_f = 8 \times 0.0032 \frac{(120)}{(25 \times 10^{-3})} 988 \times \frac{1.98^2}{2} \tag{20.1}$$

$$= 240,388 \text{ N/m}^2$$

$$\text{Total pressure} = 28,754 + 240,388 = 269,142 \text{ N/m}^2 = \underline{\underline{270 \text{ kN/m}^2}}$$

Method 2: Equivalent pipe diameters

Extra length of pipe to allow for miscellaneous losses:

$$= 735 \times 25 \times 10^{-3} = 18.4 \text{ m}$$

$$\text{So, total length for } \Delta P \text{ calculation} = 120 + 18.4 = 138.4 \text{ m}$$

$$\Delta P_f = 8 \times 0.0032 \frac{(138.4)}{(25 \times 10^{-3})} 998 \times \frac{1.98^2}{2} = 277,247 \text{ N/m}^2 \tag{20.1}$$

$$= \underline{\underline{277 \text{ kN/m}^2}}$$

Note: The two methods will not give exactly the same result. The method using velocity heads is the more fundamentally correct approach, but the use of equivalent diameters is easier to apply and sufficiently accurate for use in preliminary design calculations.

20.5 Valves

The valves used for chemical process plant can be divided into two broad classes, depending on their primary function:

1. Shut-off valves (block valves or isolation valves), whose purpose is to close off the flow
2. Control valves, both manual and automatic, used to regulate flow

The main types of valves used are:

Gate	Fig. 20.6(a)
Plug	Fig. 20.6(b)
Ball	Fig. 20.6(c)
Globe	Fig. 20.6(d)
Diaphragm	Fig. 20.6(e)
Butterfly	Fig. 20.6(f)

A valve selected for shut-off purposes should give a positive seal in the closed position and minimum resistance to flow when open. Gate, plug, and ball valves are most frequently used for this purpose. Gate valves are available in

the widest range of sizes and can be operated manually or by a motor. They have a straight-through flow channel and low pressure drop when fully open. Several turns of the valve handle are usually required to close the valve, so they are best used when operated infrequently. Gate valves should not be operated partially open, as the valve seals can become deformed, causing the valve not to seal properly. Plug valves and ball valves have the advantage in that they only require a quarter-turn to open or close. These valves are often actuated by solenoids and are used where quick on–off switching is needed. The selection of valves is discussed by Merrick (1986, 1990), Smith and Vivian (1995), and Smith and Zappe (2003).

If flow control is required, the valve should be capable of giving smooth control over the full range of flow, from fully open to closed. Globe valves are normally used, though diaphragm valves are also common. Butterfly valves are often used for the control of gas and vapor flows. Automatic control valves are usually globe valves with special trim designs (see Chhabra & Rohani, 2017).

The careful selection and design of control valves are important; good flow control must be achieved without introducing excessive pressure drop. Control valve sizing is discussed in more detail in Section 20.11.

Nonreturn valves are used to prevent back flow of fluid in a process line. They do not normally give an absolute shut-off of the reverse flow. A typical design is shown in Fig. 20.6(g). Because swing-type check valves depend on gravity to close the valve, care must be taken to orient the valve properly when locating and installing it.

Standards for valves are set by the ASME B16 Standards Committee and can be ordered from the American Society of Mechanical Engineers. General standards are described in ASME B16.34-2017, while valve dimensions are given in ASME B16.10-2017. Valve design is covered by Pearson (1978).

20.6 Compression and expansion of gases

The equipment used to compress a gas through a process piping system is different from that used for liquids. At low pressure drops, a simple fan may be adequate. At higher pressure drops, multistage compressors are commonly used. The different types of compressors were introduced in Section 20.3.1. This section discusses the sizing of compressors and estimation of the work required to compress a gas or vapor. Several textbooks are available on compressor design, selection, and operation: Bloch et al. (1982), Brown (2005), and Aungier (1999, 2003). An introduction to centrifugal compressor selection is given in the article by Sorokes (2013).

20.6.1 Compression of gases

The work done in compressing or expanding a gas or vapor is given by:

$$-W = \int_{\upsilon_1}^{\upsilon_2} P \, \mathrm{d}\upsilon \tag{20.3}$$

To calculate the work done, a relationship between pressure and volume during the expansion is needed.

If the compression or expansion is isothermal (at constant temperature), then for unit mass of an ideal gas:

$$P\upsilon = \text{constant} \tag{20.4}$$

and the work done,

$$-W = P_1 \upsilon_1 \ln \frac{P_2}{P_1} = \frac{\mathbf{R}T_1}{M_w} \ln \frac{P_2}{P_1} \tag{20.5}$$

where P_1 = initial pressure
P_2 = final pressure
υ_1 = initial volume
$\mathbf{R}$ = universal gas constant
M_w = molecular mass (weight) of gas

In industrial compressors or expanders, the compression or expansion path will be "polytropic," approximated by the expression:

$$P\upsilon^n = \text{constant} \tag{20.6}$$

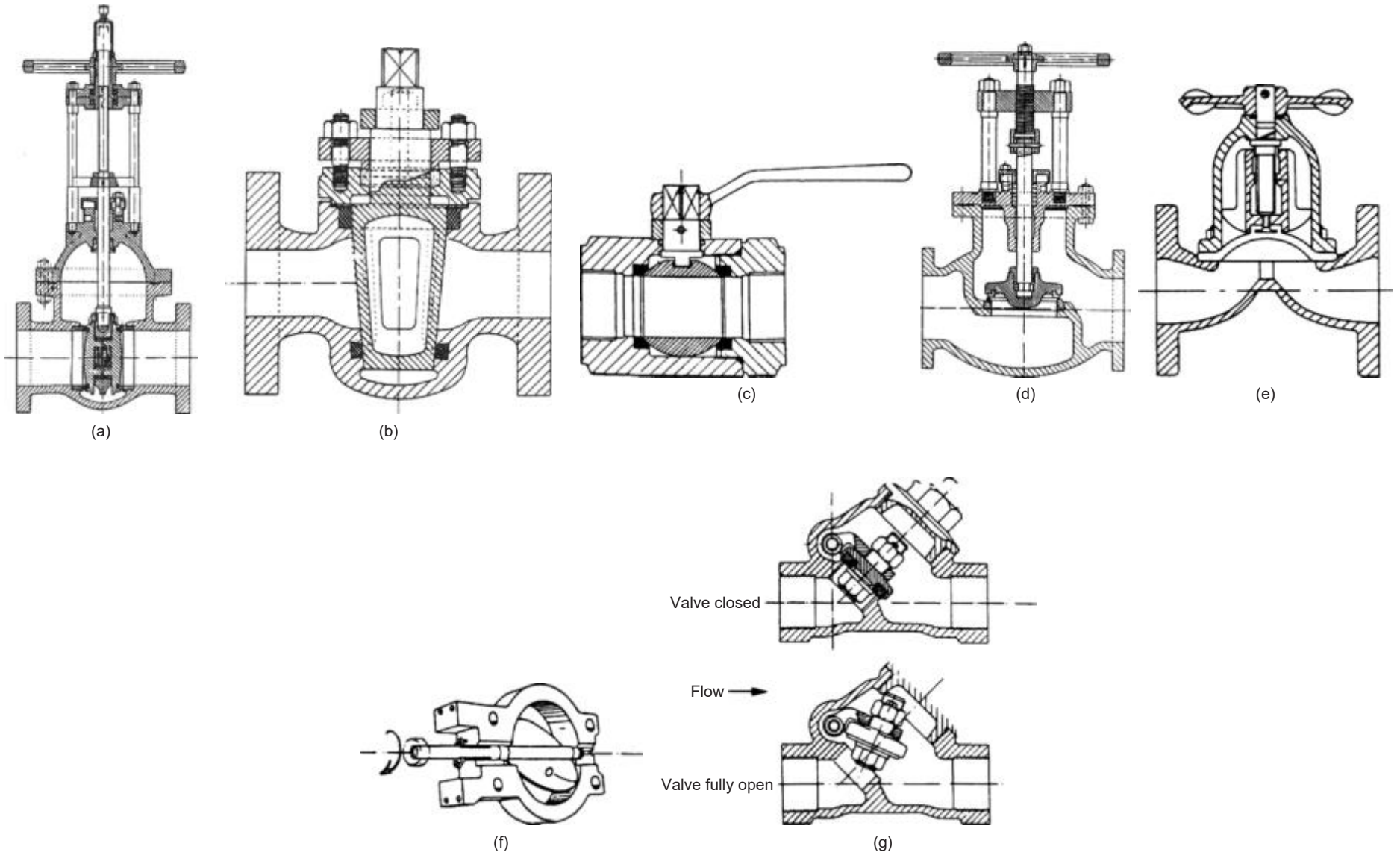


FIG. 20.6 (a) Gate valve (slide valve). (b) Plug valve. (c) Ball valve. (d) Globe valve. (e) Diaphragm valve. (f) Butterfly valve. (g) Nonreturn valve, check valve, hinged disc type.

where n is the polytropic expansion coefficient. The work produced (or required) is given by the general expression (see Chhabra & Shankar, 2017):

$$-W = P_1 v_1 \frac{n}{n-1}\left[\left(\frac{P_2}{P_1}\right)^{(n-1)/n} - 1\right] = Z\,\frac{RT_1}{M_w}\,\frac{n}{n-1}\left[\left(\frac{P_2}{P_1}\right)^{(n-1)/n} - 1\right] \tag{20.7}$$

where Z = compressibility factor (1 for an ideal gas)
$\mathbf{R}$ = universal gas constant, 8.314 JK^{-1} mol^{-1}
T_1 = inlet temperature, K
W = work done, kJ/kg

The value of n will depend on the design and operation of the machine.

The energy required to compress a gas, or the energy obtained from expansion, can be estimated by calculating the ideal work and applying a suitable efficiency value. For reciprocating compressors, the isentropic work is normally used ($n = \gamma$, where γ is the ratio of specific heats) (see Fig. 20.9), and for centrifugal or axial machines the polytropic work (see Fig. 20.8 and Section 20.6.3).

20.6.2 Mollier diagrams

If a Mollier diagram (enthalpy–pressure–temperature–entropy chart) is available for the working fluid, the isentropic work can be easily calculated.

$$W = H_1 - H_2 \tag{20.8}$$

where H_1 = the specific enthalpy at the pressure and temperature corresponding to point 1, the initial gas conditions
H_2 = the specific enthalpy corresponding to point 2, the final gas condition

Point 2 is found from point 1 by tracing a path (line) of constant entropy on the diagram.
The method is illustrated in Example 20.2.

Example 20.2

Methane is compressed from 1 bar and 290 K to 10 bar. If the isentropic efficiency is 0.85, calculate the energy required to compress 10,000 kg/h. Estimate the exit gas temperature.

Solution

From the Mollier diagram, shown diagrammatically in Fig. 20.7:

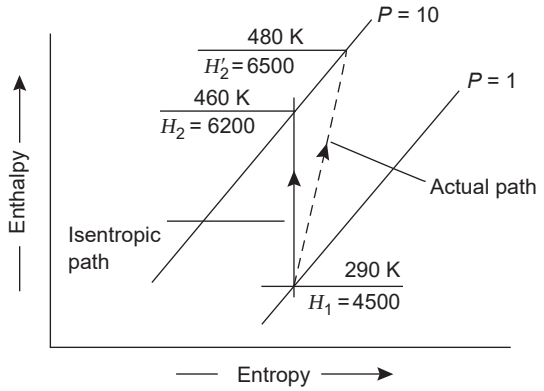


FIG. 20.7 Mollier diagram, methane.

$$H_1 = 4500 \text{ cal/mol}$$
$$H_2 = 6200 \text{ cal/mol (isentropic path)}$$
$$\text{Isentropic work} = 6200 - 4500$$
$$= \underline{\underline{1700 \text{ cal/mol}}}$$

For an isentropic efficiency of 0.85:

$$\text{Actual work done on gas } \frac{1700}{0.85} = 2000 \text{ cal/mol}$$

So, actual final enthalpy:

$$H_2' = H_1 + 2000 = \underline{\underline{6500 \text{ cal/mol}}}$$

From the Mollier diagram, if all the extra work is taken as irreversible work done on the gas, the exit gas temperature $= \underline{\underline{480 \text{ K}}}$

$$\text{Molecular weight of methane} = 16$$

$$\text{Energy required} = (\text{moles per hour}) \times (\text{specific enthalpy change})$$
$$= \frac{10,000}{16} \times 2000 \times 10^3$$
$$= 1.25 \times 10^9 \text{cal/h}$$
$$= 1.25 \times 10^9 \times 4.187 \text{ J/h}$$
$$= 5.23 \times 10^9 \text{J/h}$$
$$\text{Power} = \frac{5.23 \times 10^9}{3600} = \underline{\underline{1.45 \text{ MW}}}$$

20.6.3 Polytropic compression and expansion

If no Mollier diagram is available, it is more difficult to estimate the ideal work in compression or expansion processes.

Equation 20.7 can be used if the compressibility Z and polytropic coefficient n are known. Compressibility can be plotted against reduced temperature and pressure, as shown in Fig. 20.10.

At conditions away from the critical point:

$$n = \frac{1}{1-m} \tag{20.9}$$

where:

$$m = \frac{(\gamma - 1)}{\gamma E_p} \text{ for compression} \tag{20.10}$$

$$m = \frac{(\gamma - 1) E_p}{\gamma} \text{ for expansion} \tag{20.11}$$

and E_p is the polytropic efficiency, defined by:

$$\text{for compression } E_p = \frac{\text{polytropic work}}{\text{actual work required}}$$

$$\text{for expansion } E_p = \frac{\text{actual work obtained}}{\text{polytropic work}}$$

An estimate of E_p can be obtained from Fig. 20.8.

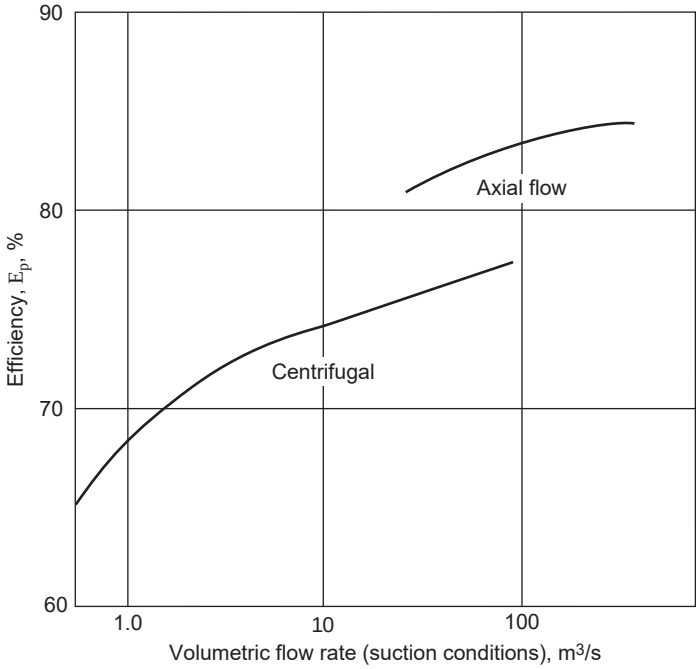


FIG. 20.8 Approximate polytropic efficiencies of centrifugal and axial-flow compressors.

The outlet temperature can be estimated from:

$$T_2 = T_1\left(\frac{P_2}{P_1}\right)^m \tag{20.12}$$

Close to the critical conditions these equations should not be used. The procedure for calculation of polytropic work of compression or expansion close to the critical point is more complex (Schultz, 1962), and it is easiest to make such calculations using process simulation programs.

Example 20.3

Estimate the power required to compress 5000 kmol/h of HCl at 5 bar, 15 °C, to 15 bar.

Solution

For HCl, critical conditions are $P_c = 82$ bar, $T_c = 324.6$ K.
Estimate T_2 from Equation 20.12. For diatomic gases $\gamma \approx 1.4$.
Note: γ could be estimated from the relationship:

$$\gamma = \frac{C_p}{C_v}$$

From Fig. 20.8, $E_p = 0.73$.
From Equation 20.10:

$$m = \frac{1.4 - 1}{1.4 \times 0.73} = 0.391$$

$$T_2 = 288\left(\frac{15}{5}\right)^{0.39} = 442 \text{ K}$$

$$T_{r(\text{mean})} = \frac{442 + 288}{2 \times 324.6} = 1.12$$

$$P_{r(\text{mean})} = \frac{5 + 15}{2 \times 82} = 0.12$$

From Fig. 20.10, at mean conditions:

$$Z = 0.98$$

From Equation 20.9:

$$n = \frac{1}{1 - 0.391} = 1.64$$

From Equation 20.7:

$$W \text{ polytropic} = 0.98 \times 288 \times 8.314 \times \frac{1.64}{1.64 - 1}\left(\left(\frac{15}{5}\right)^{(1.64-1)/1.64} - 1\right)$$

$$= \underline{\underline{3219 \text{ kJ/kmol}}}$$

$$\text{Actual work required} = \frac{\text{polytropic work}}{E_p} = \frac{3219}{0.73} = \underline{\underline{4409 \text{ kJ/kmol}}}$$

$$\text{Power} = \frac{4409 \times 5000}{3600} = 6124 \text{ kW, say } \underline{\underline{6.1 \text{ MW}}}$$

Example 20.4

Consider the extraction of energy from the tail gases from a nitric acid adsorption tower.
Gas composition, kmol/h:

O_2	371.5
N_2	10,014.7
NO	21.9
NO_2	Trace
H_2O	Saturated at 25 °C

If the gases leave the tower at 6 atm, 25 °C, and are expanded to, say, 1.5 atm, calculate the turbine exit gas temperatures, without pre-heat, and if the gases are pre-heated to 400 °C with the reactor off-gas. Also, estimate the power recovered from the pre-heated gases.

Solution

For the purposes of this calculation, it will be sufficient to consider the tail gas as all nitrogen, flow 10,410 kmol/h.

$$P_c = 33.5 \text{ atm}, T_c = 126.2 \text{ K}$$

Fig. 20.8 can be used to estimate the turbine efficiency:

$$\text{Exit gas volumetric flow rate} = \frac{10,410}{3600} \times 22.4 \times \frac{1}{1.5} \approx 43 \text{ m}^3/\text{s}$$

from Fig. 20.8 $E_P = 0.75$:

$$P_r \text{ inlet} = \frac{6}{33.5} = 0.18$$

$$T_r \text{ inlet} = \frac{298}{126.2} = 2.4$$

Using Equations 20.9 and 20.11, for N_2, $\gamma = 1.4$:

$$m = \frac{1.4-1}{1.4} \times 0.75 = 0.21$$

$$n = \frac{1}{1-m} = \frac{1}{1-0.21} = 1.27$$

$$\text{Without pre-heat } T_2 = 298\left(\frac{1.5}{6.0}\right)^{0.21} = 223 \text{ K}$$

$$= \underline{\underline{-50\ ^\circ\text{C}}}$$

This temperature would be problematic. Acidic water would condense out, probably damaging the turbine.

$$\text{With pre-heat, } T_2 = 673\left(\frac{1.5}{6.0}\right)^{0.21} = 503 \text{ K}$$

$$= \underline{\underline{230\ ^\circ\text{C}}}$$

From Equation 20.7, the work done by the gas as a result of polytropic expansion is:

$$= -1 \times 673 \times 8.314 \times \frac{1.27}{1.27-1}\left\{\left(\frac{1.5}{6.0}\right)^{(1.27-1)/1.27} - 1\right\}$$

$$= 6718 \text{ kJ/kmol}$$

$$\text{Actual work} = \text{polytropic work} \times Ep$$

$$= 6718 \times 0.75 = \underline{\underline{5039 \text{ kJ/kmol}}}$$

$$\text{Power output} = \text{work/kmol} \times \text{kmol/s} = 5039 \times \frac{10,410}{3600}$$

$$= 14,571 \text{ kJ/s} = \underline{\underline{14.6 \text{ MW}}}$$

This is a significant amount of power and will probably justify the cost of the expansion turbine.

20.6.4 Multistage compressors

Single-stage compressors can only be used for low pressure ratios. At high pressure ratios, the temperature rise is too high for efficient operation.

To cope with the need for high pressure generation, the compression is split into a number of separate stages, with intercoolers between each stage. The interstage pressures are normally selected to give equal work in each stage. For an n-stage compressor, this occurs when the compression ratio across each stage is the nth root of the overall compression ratio.

For a two-stage compressor, the interstage pressure is given by:

$$P_i = \sqrt{(P_1 \times P_2)} \tag{20.13}$$

where P_i is the intermediate-stage pressure.

Example 20.5

Estimate the power required to compress 1000 m^3/h air from ambient conditions to 700 kN/m^2 gauge, using a two-stage reciprocating compressor with an intercooler.

Solution

Take the inlet pressure, P_1, as 1 atmosphere = 101.33 kN/m^2, absolute.
Outlet pressure, P_2, = 700 + 101.33 = 801.33 kN/m^2, absolute.
For equal work in each stage, the intermediate pressure, P_i,

$$= \sqrt{(1.0133 \times 10^5 \times 8.0133 \times 10^5)} = \underline{\underline{2.8495 \times 10^5}} \text{ N/m}^2$$

For air, take ratio of the specific heats, γ, to be 1.4.
For equal work in each stage, the total work will be twice that in the first stage.
Take the inlet temperature to be 20 °C, At that temperature, the specific volume is given by:

$$v_1 = \frac{29}{22.4} \times \frac{293}{273} = 1.39 \text{ m}^3/\text{kg}$$

$$\text{Isentropic work done, } -W = 2 \times 1.0133 \times 10^5 \times 1.39 \times \frac{1.4}{1.4 - 1}\left(\left(\frac{2.8495}{1.0133}\right)^{(1.4-1)/1.4} - 1\right)$$

$$= 338,844 \text{ J/kg} = 339 \text{ kJ/kg}$$

From Fig. 20.9, for a compression ratio of 2.85, the efficiency is approximately 84%. So work required:

$$= 339/0.84 = \underline{\underline{404}} \text{ kJ/kg}$$

$$\text{Mass flow rate} = \frac{1000}{1.39 \times 3600} = 0.2 \text{ kg/s}$$

$$\text{Power required} = 404 \times 0.2 = \underline{\underline{80 \text{ kW}}}$$

20.6.5 Compressor performance curves

Multistage centrifugal compressors and axial compressors can be operated over a range of conditions by varying the compressor speed. A typical set of performance curves is shown in Fig. 20.11. The shape of the curves depends on the number of stages in the compressor. As more stages are added to the compressor, the curves become longer and flatter, approaching constant pressure head delivered for a given speed.

At low-volume flow rates, compressor operation can become unstable. If the flow rate is low, the pressure in the discharge pipe can become temporarily greater than the pressure delivered by the compressor, leading to momentary flow reversal. When the flow reverses, the outlet pressure drops and the compressor begins to deliver gas again. This causes a pulsation in outlet pressure and flow known as *surge* or *pumping*, which can cause damage to the compressor. Compressors are usually instrumented to prevent surge from occurring.

Some compressors are equipped with adjustable inlet guide vanes to further extend the range of operation by allowing the inlet flow to be throttled.

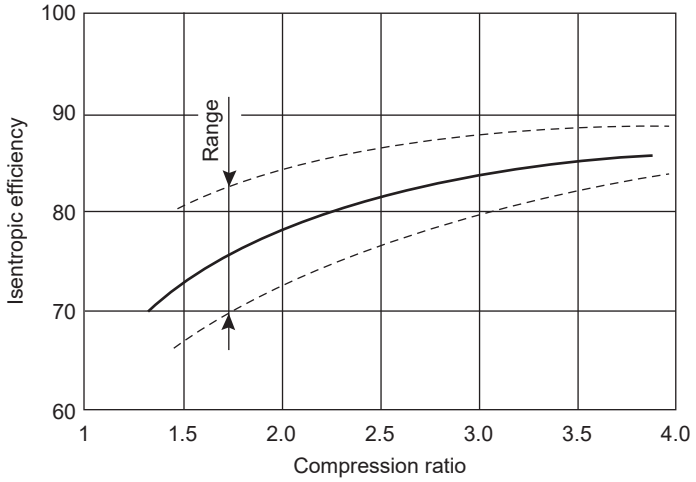


FIG. 20.9 Typical efficiencies for reciprocating compressors.

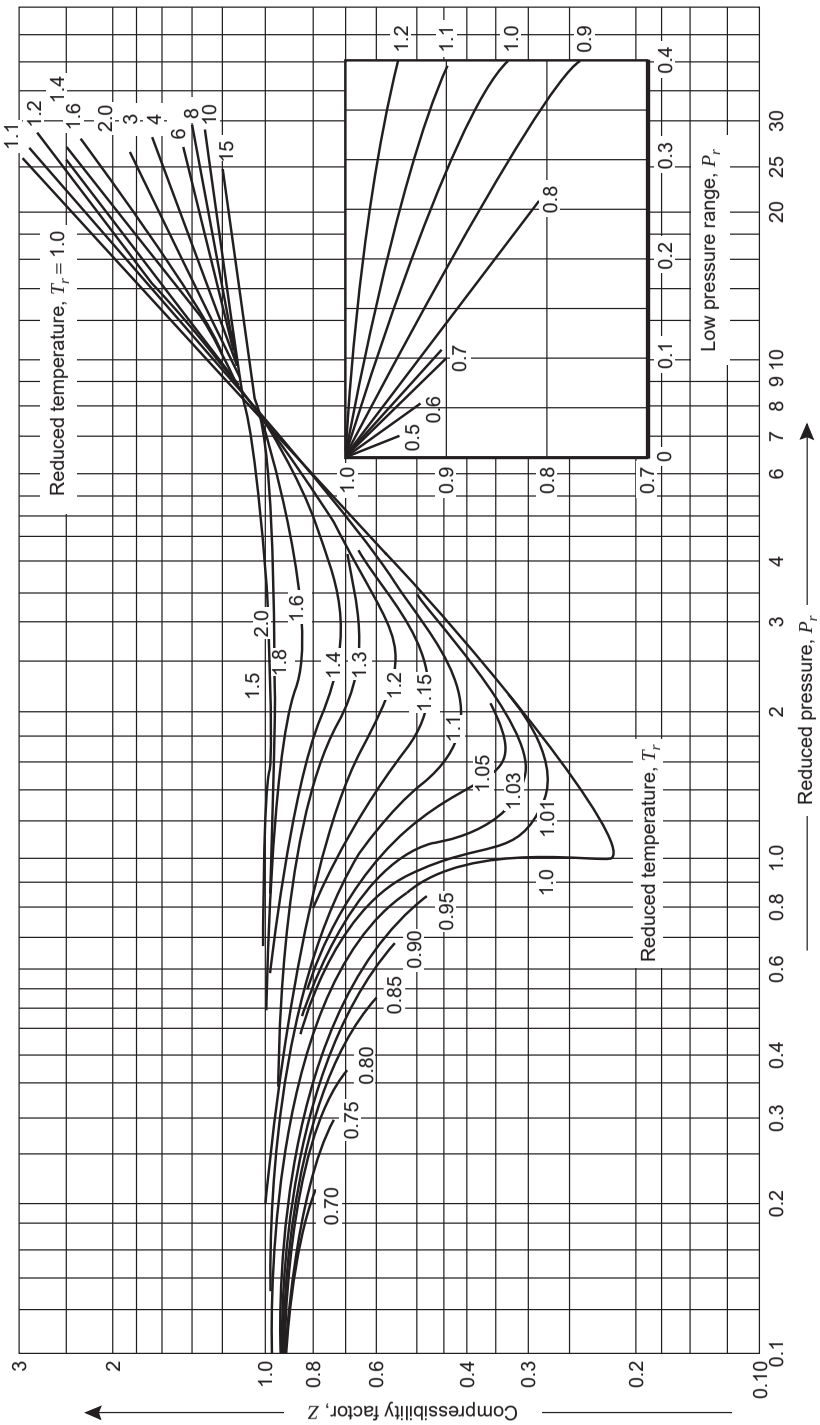


FIG. 20.10 Compressibility factors of gases and vapors.

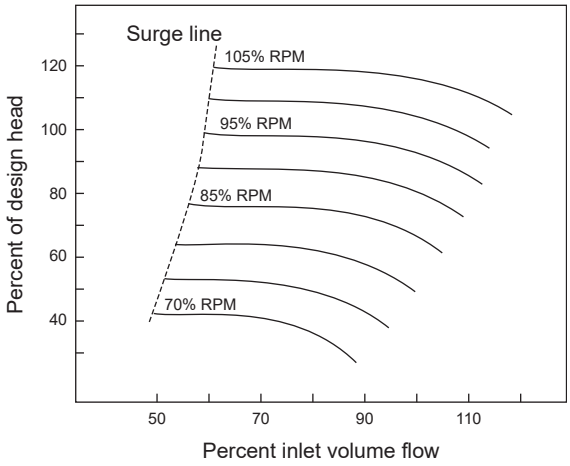


FIG. 20.11 Typical centrifugal compressor performance curves.

20.7 Pumping of liquids

The different types of pumps used for transporting liquids are introduced in Section 20.3.2. This section describes the design and selection of centrifugal pumps in more detail. Centrifugal pumps are by far the most widely used type, as they are compact, inexpensive, robust, and available in a wide range of materials.

20.7.1 Centrifugal pump design

A centrifugal pump consists of a shaped impeller with curved radial vanes, which is housed inside a casing (Fig. 20.12). A shaft connects the impeller to a power source such as an electric motor or steam turbine, which causes the impeller to rotate at high speed. Fluid enters the casing in the axial direction, towards the center of the impeller, and is pushed out towards the edge of the casing by centrifugal force. The high speed of the impeller gives the fluid a high kinetic energy, which is then converted into higher pressure as the liquid decelerates to the tangential discharge pipe.

Different types and sizes of impellers can be used with the same pump. Specialized impellers are available for pumping slurries and suspensions; see Nwaokocha (2019). The pump casing is usually designed as a volute casing, which is a spiral that increases uniformly in cross-sectional area towards the discharge. Some pumps also incorporate fixed guide vanes or diffusers between the impeller and casing, which gives a more gradual change in direction to the fluid and leads to improved efficiency.

Centrifugal pumps are characterized by their specific speed. In the dimensionless form, specific speed is given by:

$$N_s = \frac{NQ^{1/2}}{(gh)^{3/4}} \tag{20.14}$$

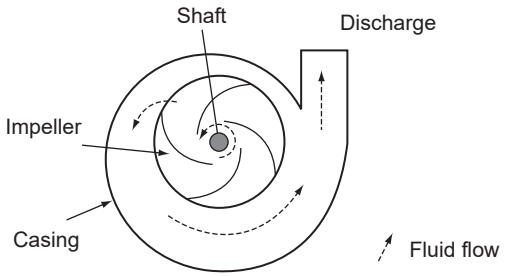


FIG. 20.12 Schematic diagram of a centrifugal pump.

where N = revolutions per second
Q = flow, m^3/s
h = head, m
g = gravitational acceleration m/s^2

Pump manufacturers do not generally use the dimensionless specific speed, but define the impeller specific speed by the equation:

$$N'_S = \frac{N' Q^{1/2}}{h^{3/4}} \tag{20.15}$$

where N' = revolutions per minute (rpm)
Q = flow, U.S. gal/min
h = head, ft

Values of the nondimensional specific speed, as defined by Equation 20.14, can be converted to the form defined by Equation 20.15 by multiplying by 1.72×10^4 $gal^{0.5}min^{-1.5}ft^{-0.75}$.

The impeller specific speed for centrifugal pumps (Equation 20.15) usually lies between 400 and 20,000, depending on the type of impeller. Generally, pump impellers are classified as centrifugal or radial for specific speeds between 400 and 4000, mixed flow between 4000 and 9000, and axial above 9000 (Heald, 2002). Doolin (1977) states that below a specific speed of 1000, the efficiency of single-stage centrifugal pumps is low and multistage pumps should be considered.

20.7.2 Power requirements for pumping liquids

To transport a liquid from one vessel to another through a pipeline, energy has to be supplied to:

1. Overcome the friction losses in the pipes
2. Overcome the miscellaneous losses in the pipe fittings (e.g., bends), valves, instruments, etc.
3. Overcome the losses in process equipment (e.g., heat exchangers, packed beds)
4. Overcome any difference in elevation from end to end of the pipe
5. Overcome any difference in pressure between the vessels at each end of the pipeline

The total energy required can be calculated from the energy equation:

$$g\Delta z + \Delta P/\rho - \Delta P_f/\rho - W = 0 \tag{20.16}$$

where W = work done by the fluid, J/kg
Δz = difference in elevations ($z_1 - z_2$), m (Fig. 20.13)
ΔP = difference in system pressures ($P_1 - P_2$), N/m^2
ΔP_f = pressure drop due to friction, including miscellaneous losses and equipment losses (see Section 20.4), N/m^2
ρ = liquid density, kg/m^3
g = acceleration due to gravity, m/s^2

If W is negative, a pump is required; if it is positive, a turbine could be installed to extract energy from the system.

$$\text{The head required from the pump} = \Delta P_f/\rho g - \Delta P/\rho g - \Delta z \tag{20.17}$$

Pump shaft power

The power required is given by:

$$\text{Power} = (W \times m) \times 100/\eta_p, \text{ for a pump} \tag{20.18}$$

where m = mass flow rate, kg/s
η_p = pump efficiency, percent

For an incompressible fluid, the power required can also be written as:

$$\text{Power} = \frac{\Delta P Q}{\eta_p} \times 100 \tag{20.19}$$

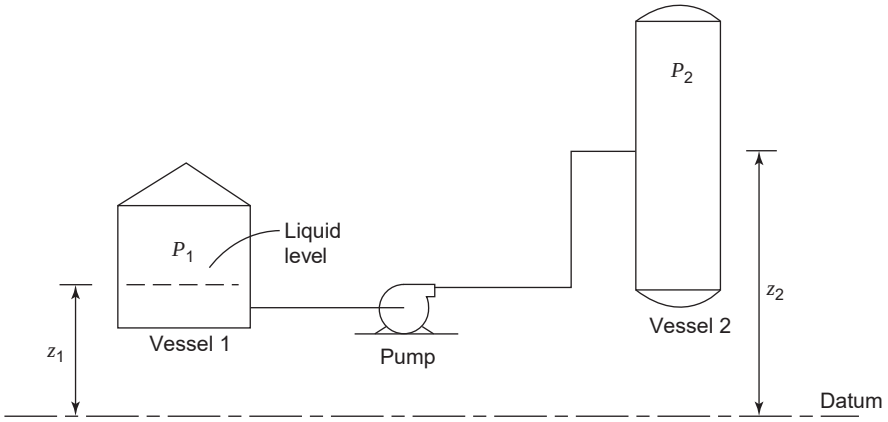


FIG. 20.13 Piping system.

where ΔP = pressure differential across the pump, N/m^2
Q = flow rate, m^3/s

The efficiency of centrifugal pumps will depend on the size and type of pump used and the operating conditions. The values given in Fig. 20.14 can be used to estimate the power and energy requirements for preliminary design purposes. The efficiency of reciprocating pumps is usually around 90%.

When a pump is used as a hydraulic power recovery turbine, the work delivered is given by:

$$\text{Power delivered} = (W \times m) \times \eta_t \tag{20.20}$$

where η_t = turbine efficiency = power out/power in.

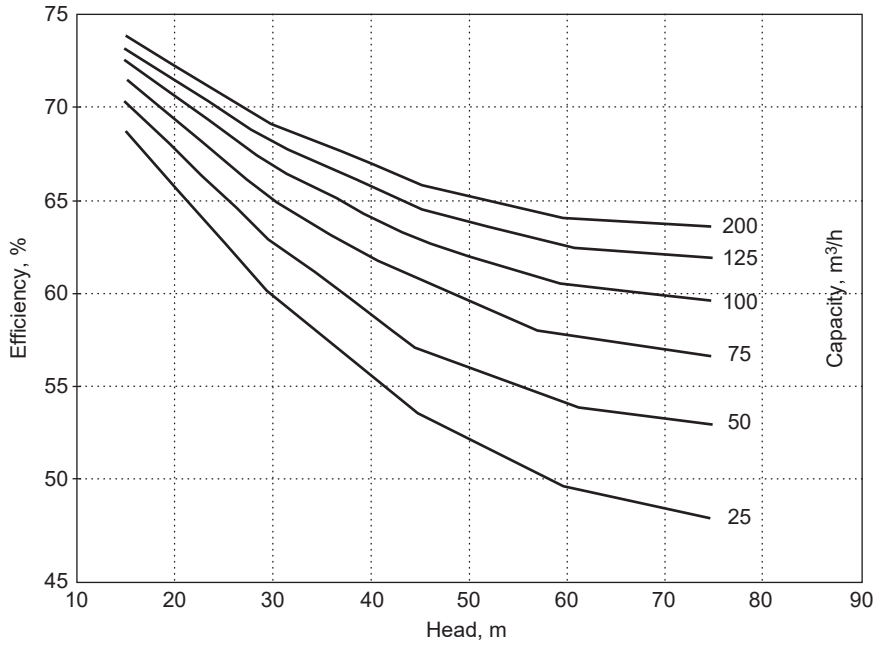


FIG. 20.14 Centrifugal pump efficiency.

Example 20.6

A tanker carrying toluene is unloaded, using the ship's pumps, to an on-shore storage tank. The pipeline is 225 mm internal diameter and 900 m long. Miscellaneous losses due to fittings, valves, etc., amount to 600 equivalent pipe diameters. The maximum liquid level in the storage tank is 30 m above the lowest level in the ship's tanks. The ship's tanks are nitrogen blanketed and maintained at a pressure of 1.05 bar. The storage tank has a floating roof, which exerts a pressure of 1.1 bar on the liquid.

The ship must unload 1000 metric tons within 5 hours to avoid demurrage charges. Estimate the power required by the pump. Take the pump efficiency as 70%.

Physical properties of toluene: density 874 kg/m^3, viscosity 0.62 mNm^{-2} s.

Solution

$$\text{Cross-sectional area of pipe} = \frac{\pi}{4}\left(225\times 10^{-3}\right)^2 = 0.0398\ \text{m}^2$$

$$\text{Minimum fluid velocity} = \frac{1000\times 10^3}{5\times 3600}\times\frac{1}{0.0398}\times\frac{1}{874} = 1.6\ \text{m/s}$$

$$\text{Reynolds number} = \left(874\times 1.6\times 225\times 10^{-3}\right)/0.62\times 10^{-3}$$

$$= 507,484 = 5.1\times 10^5 \tag{20.2}$$

Absolute roughness commercial steel pipe, Table 20.3 = 0.046 mm
Relative roughness = 0.046/225 = 0.0002
Friction factor from Fig. 20.5, $f = 0.0019$
Total length of pipeline, including miscellaneous losses:

$$= 900 + 600\times 225\times 10^{-3} = 1035\ \text{m}$$

Friction loss in pipeline,

$$\Delta P_f = 8\times 0.0019\times\left(\frac{1035}{225\times 10^{-3}}\right)\times 874\times\frac{1.62^2}{2}$$

$$= 78,221\ \text{N/m}^2$$

Maximum difference in elevation, $(z_1 - z_2) = (0-30) = \underline{\underline{-30\ \text{m}}}$

Pressure difference, $(P_1 - P_2) = (1.05-1.1)10^5 = \underline{\underline{-5\times 10^3}}\ \text{N/m}^2$ (20.1)

Energy balance:

$$9.8(-30) + (-5\times 103)/874 - (78,221)/874 - W = 0$$

$$W = \underline{\underline{-389.2}}\ \text{J/kg} \tag{20.16}$$

$$\text{Power} = (389.2\times 55.56)/0.7 = 30,981\ \text{W}, \quad \text{say } \underline{\underline{31\ \text{kW.}}} \tag{20.18}$$

Note that this is the maximum power required by the pump at the end of the unloading when the ship's tank is nearly empty and the storage tank is nearly full. Initially, the difference in elevation is lower and the power required is reduced. For design purposes, the maximum power case would be the governing case and would be used to size the pump and motor.

20.7.3 Characteristic curves for centrifugal pumps

The performance of a centrifugal pump is characterized by plotting the head developed against the flow rate. The pump efficiency can be shown on the same curve. A typical plot is shown in Fig. 20.15. The head developed by the pump falls as the flow rate is increased. The efficiency rises to a maximum and then falls.

For a given type and design of pump, the performance will depend on the impeller diameter, the pump speed, and the number of stages. Pump manufacturers publish families of operating curves for the range of pumps they sell, corresponding to different combinations of casing and impeller sizes. These can be used to select the best pump for a given duty. A typical set of curves is shown in Fig. 20.16.

Pump characteristic curves are usually plotted in terms of the head delivered by the pump instead of pressure difference. A centrifugal pump will deliver the same head for any liquid of viscosity less than about 50 mNs/m^2 (50 cP). The pressure rise delivered by the pump depends on the liquid density. The design engineer should check with the pump vendor when specifying a pump for a high-viscosity liquid, a non-Newtonian liquid, or a suspension. A good guide to reading pump curves is given by Kelly (2010).

20.7.4 Cavitation and net positive suction head (NPSH)

The pressure at the inlet to a pump must be high enough to prevent cavitation from occurring in the pump. Cavitation occurs when bubbles of vapor, or gas, form in the pump casing. Vapor bubbles will form if the pressure falls below the vapor pressure of the liquid. These bubbles subsequently collapse, creating localized shock waves that cause noise and can lead to damage to the pump.

The net positive suction head available ($NPSH_{avail}$) is the pressure at the pump suction, above the vapor pressure of the liquid, expressed as head of liquid.

The net positive head required ($NPSH_{reqd}$) is a function of the design parameters of the pump and will be specified by the pump manufacturer. As a general guide, the NPSH should be above 3 m for pump capacities up to 100 m^3/h and 6 m above this capacity. Special impeller designs can be used to overcome problems of low suction head; see Doolin (1977). The NPSH required varies with flow rate and is sometimes indicated on pump characteristic curves.

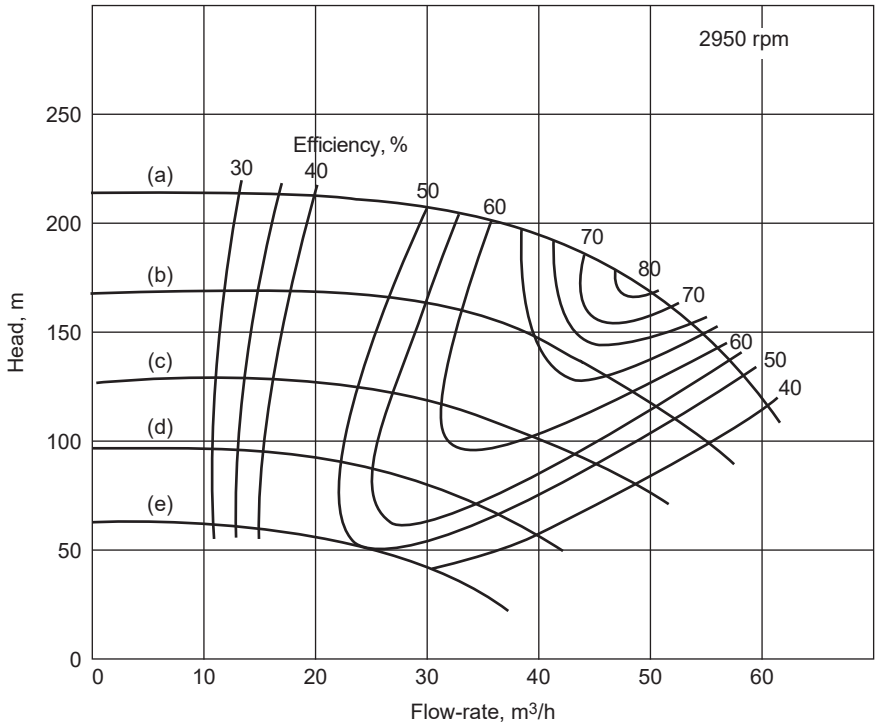


FIG. 20.15 Pump characteristics for a range of impeller sizes. (a) 250 mm. (b) 225 mm. (c) 200 mm. (d) 175 mm. (e) 150 mm.

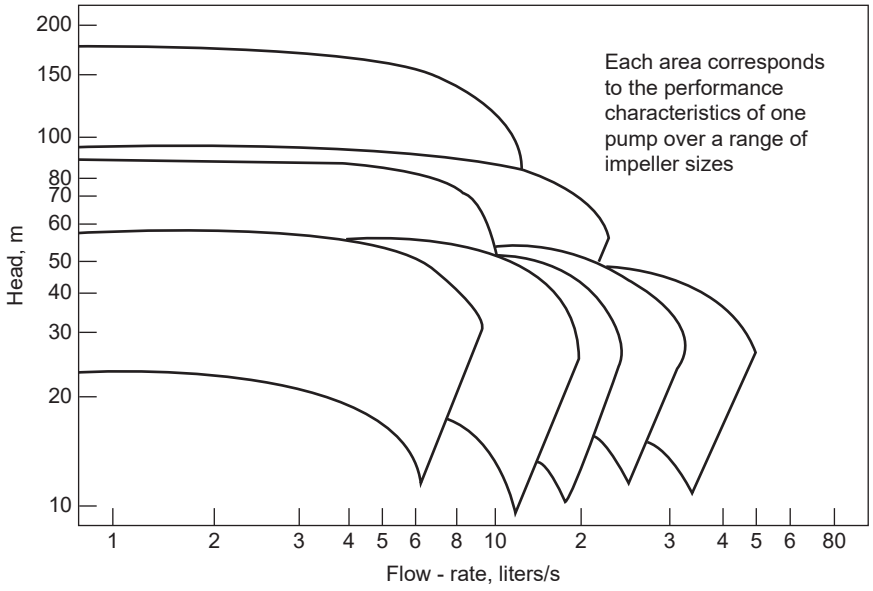


FIG. 20.16 Family of pump curves.

The net positive head available is given by the following equation:

$$\mathrm{NPSH_{avail}} = \mathrm{P}/\rho.\mathrm{g} + \mathrm{H} - \mathrm{P_f}/\rho.\mathrm{g} - \mathrm{P_v}/\rho.\mathrm{g} \tag{20.21}$$

where $NPSH_{avail}$ = net positive suction head available at the pump suction, m
P = the pressure above the liquid in the feed vessel, N/m^2
H = the height of liquid above the pump suction, m
P_f = the pressure loss in the suction piping, N/m^2
P_v = the vapor pressure of the liquid at the pump suction, N/m^2
ρ = the density of the liquid at the pump suction temperature, kg/m^3
g = the acceleration due to gravity, m/s^2

The inlet piping arrangement must be designed to ensure that $NPSH_{avail}$ exceeds $NPSH_{reqd}$ under all operating conditions.

The calculation of $NPSH_{avail}$ is illustrated in Example 20.7.

Example 20.7

Liquid chlorine is unloaded from rail tankers into a storage vessel. To provide the necessary NPSH, the transfer pump is placed in a pit below ground level. Given the following information, calculate the NPSH available at the inlet to the pump at a maximum flow rate of 16,000 kg/h.

The total length of the pipeline from the rail tanker outlet to the pump inlet is 50 m. The vertical distance from the tank outlet to the pump inlet is 10 m. Commercial steel piping, 50 mm internal diameter, is used.

Miscellaneous friction losses due to the tanker outlet constriction and the pipe fittings in the inlet piping are equal to 1000 equivalent pipe diameters. The vapor pressure of chlorine at the maximum temperature reached at the pump is 685 kN/m^2 and its density and viscosity, 1286 kg/m^3 and 0.364 mNm^{-2} s. The pressure in the tanker is 7 bara.

Solution

Friction losses

$$\text{Miscellaneous losses} = 1000 \times 50 \times 10^{-3} = 50 \text{ m of pipe}$$

$$\text{Total length of inlet piping} = 50 + 50 = 100 \text{ m}$$

$$\text{Relative roughness, } e/d = 0.046/50 = 0.001$$

$$\text{Pipe cross-sectional area} = \frac{\pi}{4}(50 \times 10^{-3})^2 = 1.96 \times 10^{-3} \text{ m}^2 \tag{20.2}$$

$$\text{Velocity, } u = \frac{16{,}000}{3600} \times \frac{1}{1.96 \times 10^{-3}} \times \frac{1}{1286} = 1.76 \text{ m/s}$$

$$\text{Reynolds number} = \frac{1286 \times 1.76 \times 50 \times 10^{-3}}{0.364 \times 10^{-3}} = 3.1 \times 10^5$$

Friction factor from Fig. 20.5, $f = 0.00225$:

$$\Delta P_f = 8 \times 0.00225 \frac{(100)}{(50 \times 10^{-3})} \times 1286 \times \frac{1.76^2}{2} = 71{,}703 \text{ N/m}^2 \tag{20.1}$$

$$NPSH = \frac{7 \times 10^5}{1286 \times 9.8} + 10 - \frac{71.703}{1286 \times 9.8} - \frac{685 \times 10^3}{1286 \times 9.8} \tag{20.21}$$

$$= 55.5 + 10 - 5.7 - 54.4 = \underline{\underline{5.4 \text{ m}}}$$

20.7.5 System curve (operating line)

There are two components to the pressure head that have to be supplied by the pump in a piping system:

1. The static pressure, to overcome the differences in head (height) and pressure
2. The dynamic loss due to friction in the pipe, the miscellaneous losses, and the pressure loss through equipment

The static pressure difference will be independent of the fluid flow rate. The dynamic loss will increase as the flow rate is increased. It will be roughly proportional to the flow rate squared; see Equation 20.1. The system curve, or operating line, is a plot of the total pressure head versus the liquid flow rate. The operating point of a centrifugal pump can be found by plotting the system curve on the pump's characteristic curve; see Example 20.8. The operating point is the point where the system curve and pump curve intersect.

When selecting a centrifugal pump for a given duty, it is important to match the pump characteristic with the system curve. The operating point should be as close as is practical to the point of maximum pump efficiency, allowing for the range of flow rate over which the pump may be required to operate. This requires a good understanding of the pressure drop across the control valve if a valve is used in the line downstream of the pump. The control valve pressure drop will be proportional to the velocity squared and can range from as low as 6 to over 100 velocity heads over the range of operation of the valve, depending on the type of valve chosen (see Table 20.4). The system curve should be plotted for the case when the valve is fully open and the case when the valve is quarter-open (or at the minimum fraction open recommended by the valve manufacturer) to determine the range over which flow can be controlled with a given combination of valve and pump. Details of valve pressure drop can be obtained from manufacturers.

Most centrifugal pumps are controlled by throttling the flow with a valve on the pump discharge. This varies the dynamic pressure loss, and thus the position of the operating point on the pump characteristic curve. Throttling the flow causes an energy loss. This energy loss is acceptable in most applications; however, when the flow rates are large, the use of variable-speed control on the pump drive should be considered as a means of conserving energy.

Methods for calculating the pressure drop through pipes and fittings are given in Section 20.4. It is important that a proper analysis is made of the system, and the use of a calculation form (worksheet) to standardize pump-head calculations is recommended. A standard calculation form ensures that a systematic method of calculation is used and provides a checklist to ensure that all the usual factors have been considered. It is also a permanent record of the calculation. A template for a standard pump and line calculation is given in Appendix G and can be downloaded in Microsoft Excel format from www.elsevier.com/books-and-journals/book-companion/9780128211793. Example 20.12 has been set out using this calculation form. The calculation should include a check on the NPSH available; see Section 20.7.4.

A more detailed discussion of the operating characteristics of centrifugal and other types of pumps is given by Couper et al. (2012) and Karassik et al. (2007).

Example 20.8

A process liquid is pumped from a storage tank to a distillation column using a centrifugal pump. The pipeline is 80 mm internal diameter commercial steel pipe, 100 m long. Miscellaneous losses are equivalent to 600 pipe diameters. The storage tank operates at atmospheric pressure and the column at 1.7 bara. The lowest liquid level in the tank will be 1.5 m above the pump inlet, and the feed point to the column is 3 m above the pump inlet.

Plot the system curve on the pump characteristic given in Fig. 20.17 and determine the operating point and pump efficiency.

Properties of the fluid: density 900 kg/m^3, viscosity 1.36 mN m^{-2}s.

Solution

Static head

Difference in elevation, $\Delta z = 3.0 - 1.5 = 1.5$ m

Difference in pressure, $\Delta P = (1.7 - 1.013)10^5 = 0.7 \times 10^5 \text{N/m}^2$

as head of liquid $= (0.7 = 10^5)/(900 \times 9.8) = 7.9$ m

Total static head $= 1.5 + 7.9 = \underline{9.4 \text{ m}}$

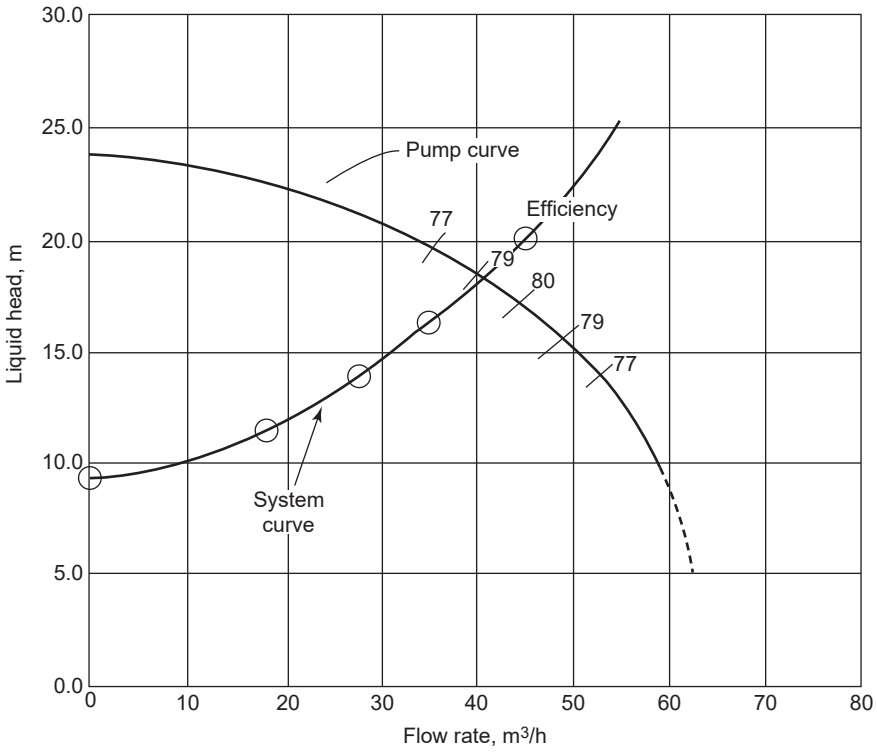


FIG. 20.17 Example 20.8.

Dynamic head

As an initial value, take the fluid velocity as 1 m/s, a reasonable value.

$$\text{Cross-sectional area of pipe} = \frac{\pi}{4}\left(80\times 10^{-3}\right)^2 = 5.03\times 10^{-3}\ \text{m}^2$$

$$\text{Volumetric flow rate} = 1\times 5.03\times 10^{-3}\times 3600 = 18.1\ \text{m}^3/\text{h} \tag{20.2}$$

$$\text{Reynolds number} = \frac{900\times 1\times 80\times 10^{-3}}{1.36\times 10^{-3}} = 5.3\times 10^4$$

$$\text{Relative roughness} = 0.046/80 = 0.0006$$

$$\text{Friction factor from Fig. 20.5}, f = 0.0027$$

$$\text{Length including miscellaneous losses} = 100 + \left(600\times 80\times 10^{-3}\right) = 148\ \text{m}$$

$$\text{Pressure drop, } \Delta P_f = 8\times 0.0027\frac{(148)}{\left(80\times 10^{-3}\right)}\times 900\times\frac{1^2}{2} = \underline{\underline{17{,}982\ \text{N/m}^2}} \tag{20.1}$$

$$= 17{,}982/(900\times 9.8) = \underline{\underline{2.03}}\ \text{m liquid}$$

$$\text{Total head} = 9.4 + 2.03 = 11.4\ \text{m}$$

To find the system curve, the calculations were repeated for the velocities shown in the following table:

Velocity m/s	Flow rate m^3/h	Static head m	Dynamic head m	Total head m
1	18.1	9.4	2.0	11.4
1.5	27.2	9.4	4.3	14.0
2.0	36.2	9.4	6.8	16.2
2.5	45.3	9.4	10.7	20.1
3.0	54.3	9.4	15.2	24.6

Plotting these values on the pump characteristic gives the operating point as 18.5 m at 41 m^3/h and the pump efficiency as 79%.

20.7.6 Pump and other shaft seals

A seal must be made where a rotating shaft passes through the casing of a pump or the wall of a vessel. The seal must serve several functions:

1. To keep the liquid contained
2. To prevent ingress of incompatible fluids, such as air
3. To prevent escape of flammable or toxic materials

Packed glands

The simplest, and oldest, form of seal is the packed gland, or stuffing box (Fig. 20.18). Its applications range from sealing the stems of the water faucets in every home to providing the seal on industrial pump, agitator, and valve shafts.

The shaft runs through a housing (gland), and the space between the shaft and the wall of the housing is filled with rings of packing. A gland follower is used to apply pressure to the packing to ensure that the seal is tight. Proprietary packing materials are used. A summary of the factors to be considered in the selection of packing materials for packed glands is given by Hoyle (1978). To make a completely tight seal, the pressure on the packing must be two to three times the system pressure. This can lead to excessive wear on rotating shafts, and lower pressures are used, allowing some leakage, which lubricates the packing. Packed glands should therefore only be specified for fluids that are not toxic, corrosive, or flammable.

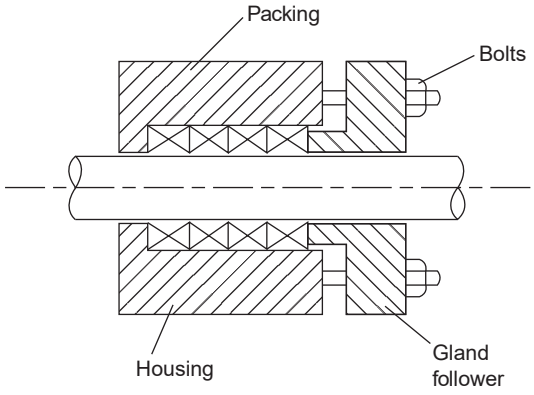


FIG. 20.18 Packed gland.

To provide positive lubrication, a lantern ring is often incorporated in the packing and lubricant forced through the ring into the packing (Fig. 20.19). With a pump seal, a flush is often taken from the pump discharge and returned to the seal, through the lantern ring, to lubricate and cool the packing. If any leakage to the environment must be avoided, a separate flush liquid can be used. A liquid must be selected that is compatible with the process fluid and the environment; water is often used.

Mechanical seals

In the process industries the conditions at the pump seal are often harsh, and more complex seals are needed. Mechanical face seals are used (Fig. 20.20). They are generally referred to simply as mechanical seals and are used only on rotating shafts.

The seal is formed between two flat faces set perpendicular to the shaft. One face rotates with the shaft; the other is stationary. The seal is made, and the faces lubricated, by a very thin film of liquid, about 0.0001 μm thick. A particular advantage of this type of seal is that it can provide a very effective seal without causing any wear on the shaft. The wear is transferred to the special seal faces. Some leakage will occur, but it is small, normally only a few drops per hour. Unlike a packed gland, a mechanical seal, when correctly installed and maintained, can be considered leak-tight.

A great variety of mechanical seal designs are available, and seals can be found to suit virtually all applications. Only the basic mechanical seal is described here. Full details and specifications of the range of seals available and their applications can be obtained from manufacturers' catalogs.

The basic mechanical seal

The components of a mechanical seal (see Fig. 20.20) are:

1. A stationary sealing ring (mating ring)
2. A seal for the stationary ring, usually O-rings or gaskets
3. A rotating seal ring (primary ring), mounted so that it can slide along the shaft to take up wear in the seal faces
4. A secondary seal for the rotating ring mount, usually O-rings or chevron seals
5. A spring to maintain contact pressure between the seal faces to push the faces together
6. A thrust support for the spring, either a collar keyed to the shaft or a step in the shaft

The assembled seal is fitted into a gland housing (stuffing box) and held in place by a retaining ring (gland plate).

Mechanical seals are classified as inside or outside, depending on whether the primary (rotating ring) is located inside the housing, running in the fluid, or outside. Outside seals are easier to maintain, but inside seals are more commonly used in the process industries, as it is easier to lubricate and flush this type. Fig. 20.20 illustrates an inside seal.

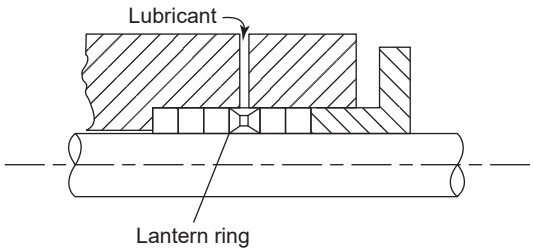


FIG. 20.19 Packed gland with lantern ring.

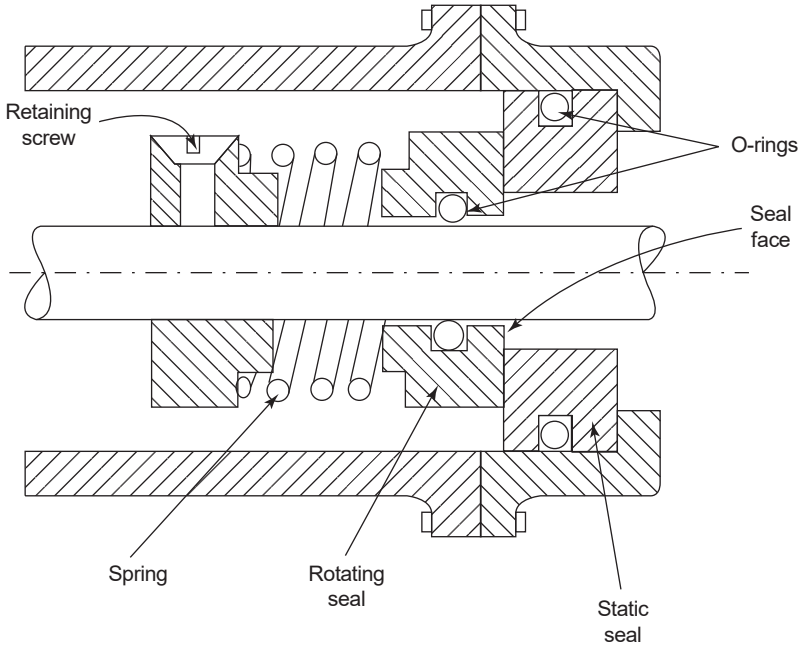


FIG. 20.20 Basic mechanical seal.

Double seals

Where it is necessary to prevent any leakage of fluid to the atmosphere, a double mechanical seal is used. The space between the two seals is flushed with a harmless fluid, compatible with the process fluid, and provides a buffer between the two seals.

Seal-less pumps (canned pumps)

Pumps that have no seal on the shaft between the pump and the drive motor are available. They are used for severe duties, where it is essential that there is no leakage into the process fluid or the environment.

The drive motor and pump are enclosed in a single casing, and the stator windings and armature are protected by metal cans; they are usually referred to as canned pumps. The motor runs in the process fluid. The use of canned pumps to control environmental pollution is discussed by Webster (1979).

20.8 Selection of drivers for rotating equipment

A mechanical driver is required to provide the shaft work to operate a pump or compressor. Electric motors are used for most small pumps, fans, and compressors, as well as most positive displacement pumps. Large compressors and pumps are sometimes powered by steam turbines. Large reciprocating compressors are occasionally powered by stand-alone diesel engines. Some axial compressors are powered by integral shaft gas turbine engines.

20.8.1 Electric motors as drivers

Alternating current electric motors are the most widely used drivers for pumps, compressors, agitators, conveyors, and most other process equipment that requires a mechanical drive. Constant-speed motors are most common, but variable-speed drivers are gaining in popularity, as they are more energy efficient. Electric motors are commercially available up to 10 MW, but special electrical infrastructure is needed for the larger sizes.

The electric power required to drive a compressor or pump can be calculated using the motor efficiency:

$$\text{Power} = \frac{-W \times m}{E_e} \tag{20.22}$$

where $-W$ = work of compression per unit mass
m = mass flow rate
E_e = electric motor efficiency

The efficiency of the drive motor will depend on the type, speed, and size. The values given in Table 20.5 can be used to make a rough estimate of the power required.

20.8.2 Steam turbines as drivers

Steam turbines are used as drivers when the process equipment requires a moderately high shaft work input, between about 1 MW and 20 MW, and when sufficient process steam is available. The use of steam turbines allows conversion of process waste heat to mechanical work, which reduces electricity costs and demands on the site electrical infrastructure.

Three main types of steam turbines are used:

- **Condensing turbines:** The downstream pressure is set by a condenser that condenses all of the steam, giving a high pressure ratio and high power per unit flow.
- **Noncondensing** or **back-pressure turbines:** The outlet pressure is controlled at a level above atmospheric pressure, usually equal to the pressure of one of the levels of the steam system so that the discharge steam can be used for process heating.
- **Extraction turbines:** Part of the steam is extracted at intermediate pressure after one or more stages of expansion, while the remainder is expanded to a condenser.

Extraction turbines allow some flexibility in meeting variations in process power and heat requirements.

The steam consumption of a steam turbine driver can be calculated by energy balance between the steam inlet and outlet conditions. Specific enthalpies of steam and condensate are given in steam tables. This calculation was illustrated in Example 3.2.

Steam turbine efficiency varies from about 60% for smaller turbines to about 85% for the larger machines.

TABLE 20.5 Approximate efficiencies of electric motors

Size (kW)	Efficiency (%)
5	80
15	85
75	90
200	92
750	95
>4000	97

20.9 Mechanical design of piping systems

20.9.1 Piping system design codes

The most widely used international design codes for pressure piping are those set by the ASME B31 Committee. Different standards are required for different services, as shown in Table 20.6. Most chemical plant and oil refinery piping is designed in accordance with ASME B31.3, which will be used as a reference in the following sections. The ASME B31.3 code applies to piping for raw, intermediate, and finished chemicals; petroleum products; gas, steam, air, and water; fluidized solids; refrigerants; and cryogenic fluids. It does not apply to:

1. Piping systems designed for pressures less than 15 psi gauge that handle fluids that are nonflammable, nontoxic, and not damaging to human tissues and are at temperatures between −29 °C (−20 °F) and 186 °C (366 °F).
2. Power boiler piping that conforms to ASME B31.1 and power boilers that conform to ASME Boiler and Pressure Vessel Code Section I.
3. Fired heater tubes, tube headers, and manifolds that are internal to the heater enclosure.
4. Internal piping and external pipe connections of pressure vessels, heat exchangers, pumps, compressors, and other fluid-handling or process equipment.

Note, though, that different design standards apply for refrigeration plants, fuel gas piping, hydrogen pipelines, power plant, and slurry-handling systems.

20.9.2 Wall thickness: Pipe schedule

The pipe wall thickness is selected to resist the internal pressure, with allowances for corrosion, erosion, and other mechanical allowances for pipe threads, etc. Process pipes can normally be considered thin cylinders; only high-pressure pipes, such as high-pressure steam lines, are likely to be classified as thick cylinders and must be given special consideration (see Chapter 14).

The ASME B31.3 code gives the following formula for pipe thickness:

$$t_m = t_p + c$$
$$t_p = \frac{P\,d}{2(SE + P\gamma_T)} \tag{20.23}$$

where t_m = minimum required thickness

TABLE 20.6 ASME pipe codes

Code no.	Scope	Latest revision
B31.1	Power piping	2018
B31.2	Fuel gas piping (withdrawn)	1968
B31.3	Process piping	2018
B31.4	Pipeline transportation systems for liquid hydrocarbons and other liquids	2019
B31.5	Refrigeration piping and heat transfer components	2016
B31.8	Gas transmission and distribution piping systems	2018
B31.9	Building services piping	2017
B31.11	Slurry transportation piping systems (superseded by ASME B31.4)	2002
B31.12	Hydrogen piping and pipelines	2014

t_p = pressure design thickness
c = sum of mechanical allowances (thread depth) plus corrosion and erosion allowances
P = internal design gauge pressure, lb/in^2 (or N/mm^2)
d = pipe outside diameter
S = basic allowable stress for pipe material, lb/in^2 (or N/mm^2)
E = casting quality factor
γ_T = temperature coefficient

Allowable stresses and values of the coefficients for different materials are given in Appendix A of the design code. Standard dimensions for stainless steel pipe are given in ASME B36.19M and for wrought steel and wrought iron pipe in ASME B36.10M. Standard pipe dimensions are also summarized by Green and Southard (2018).

Pipes are often specified by a schedule number (based on the thin cylinder formula). The schedule number is defined by:

$$\text{Schedule number} = \frac{P_s \times 1000}{\sigma_s} \tag{20.24}$$

P_s = safe working pressure, lb/in^2 (or N/mm^2)
σ_s = safe working stress, lb/in^2 (or N/mm^2)

Schedule 40 pipe is commonly used for general-purpose applications at low pressures (below 50 bar).

Example 20.9

Estimate the safe working pressure for a 4 in. (100 mm) dia., schedule 40 pipe, SA53 carbon steel, butt welded, working temperature 100 °C. The maximum allowable stress for butt welded steel pipe up to 120 °C is 11,700 lb/in^2 (79.6 N/mm^2).

Solution

$$P_S = \frac{(\text{schedule no.}) \times \sigma_S}{1000} = \frac{40 \times 11700}{1000} = \underline{468 \text{ lb/in}^2} = \underline{3180 \text{ kN/m}^2}$$

20.9.3 Pipe supports

Over long runs, between buildings and equipment, pipes are usually carried on pipe racks. These carry the main process and service pipes and are laid out to allow easy access to the equipment.

Various designs of pipe hangers and supports are used to support individual pipes. Details of typical supports can be found in the books by Green and Southard (2018) and Nayyar (2000). Pipe supports should incorporate provision for thermal expansion.

20.9.4 Pipe fittings

Pipe runs are normally made up of lengths of pipe incorporating standard fittings for joints, bends, and tees. Joints are usually welded, but small sizes may be screwed. Flanged joints are used where this is a more convenient method of assembly or if the joint will have to be frequently broken for maintenance. Flanged joints are normally used for the final connection to the process equipment, valves, and ancillary equipment.

Details of the standard pipe fittings, welded, screwed, and flanged, can be found in manufacturer's catalogues and in the appropriate national standards. Standards for pipe fittings are set by the ASME B16 committee. The standards for metal pipes and fittings are discussed by Masek (1968). Flanges and flange standards are discussed in Section 14.10.

20.9.5 Pipe stressing

Piping systems must be designed so as not to impose unacceptable stresses on the equipment to which they are connected.

Loads arise from:

1. Thermal expansion of the pipes and equipment
2. The weight of the pipes, their contents, insulation, and any ancillary equipment
3. The reaction to the fluid pressure drop
4. Loads imposed by the operation of ancillary equipment, such as relief valves
5. Vibration

Thermal expansion is a major factor to be considered in the design of piping systems. The reaction load due to pressure drop will normally be negligible. The dead-weight loads can be carried by properly designed supports.

Flexibility is incorporated into piping systems to absorb the thermal expansion. A piping system will have a certain amount of flexibility due to the bends and loops required by the layout. If necessary, expansion loops, bellows, and other special expansion devices can be used to take up expansion.

A discussion of the methods used for the calculation of piping flexibility and stress analysis is beyond the scope of this book. Manual calculation techniques, and the application of computers in piping stress analysis, are discussed in the handbook edited by Nayyar (2000).

20.9.6 Layout and design

An extensive discussion of the techniques used for piping system design and specification is beyond the scope of this book. The subject is covered thoroughly in the books by Kentish (1982a, 1982b), Lamit (1981), Parisher (2011), Whistance and Sherwood (2009), Silowash (2009), and Beale and Bowers (2017). The piping layout should generally attempt to make connections between vessels using the shortest length of pipe with the fewest bends possible, subject to the constraints of supporting the pipe, allowing for thermal expansion and providing open access for operators and maintenance.

20.10 Pipe size selection

If the motive power to drive the fluid through the pipe is available free, for instance when pressure is let down from one vessel to another or if there is sufficient head for gravity flow, the smallest pipe diameter that gives the required flow rate would normally be used. If the fluid has to be pumped through the pipe, the size should be selected to give the smallest total annualized cost.

Typical pipe velocities and allowable pressure drops that can be used to estimate pipe sizes are given here:

	Velocity m/s	ΔP kPa/m
Liquids, pumped (not viscous)	1–3	0.5
Liquids, gravity flow	—	0.05
Gases and vapors	15–30	0.02% of line pressure
High-pressure steam, >8 bar	30–60	—

Rase (1953) gives expressions for design velocities in terms of the pipe diameter. His expressions, converted to SI units, are:

Pump discharge	$0.06d_i + 0.4$ m/s
Pump suction	$0.02d_i + 0.1$ m/s
Steam or vapor	$0.2d_i$ m/s

where d_i is the internal diameter in mm.

Simpson (1968) gives values for the optimum velocity in terms of the fluid density. His values, converted to SI units and rounded, are:

Fluid density kg/m^3	Velocity m/s
1600	2.4
800	3.0
160	4.9
16	9.4
0.16	18.0
0.016	34.0

The maximum velocity should be kept below that at which erosion is likely to occur. For gases and vapors, the velocity cannot exceed the critical velocity (sonic velocity) (see Section 10.9.3 and Chhabra & Shankar (2017)) and would normally be limited to 30% of the critical velocity. Kern (1975) discusses the practical design of pump suction piping in a series of articles on the practical aspects of piping system design published in the journal *Chemical Engineering* from December 1973 to November 1975. A detailed presentation of pipe-sizing techniques is also given by Simpson (1968), who covers liquid, gas, and two-phase systems.

Economic pipe diameter

The capital cost of a pipe run increases with diameter, whereas the pumping costs decrease with increasing diameter. The most economic pipe diameter will be the one that gives the lowest total annualized cost.

A rule of thumb for the economic pipe diameter that is widely used in oil refining is:

$$\text{Economic diameter in inches} = (\text{flow rate in gpm})^{0.5}$$

In metric units this converts to:

$$d_i, \text{optimum} = 0.33(m/\rho)^{0.5}$$

where m = mass flow rate, kg/s
ρ = density, kg/m^3
d_i = pipe inside diameter, m

The formulae developed in this section are presented as an illustration of a simple optimization problem in design and to provide an estimate of economic pipe diameter in SI units. The method used is essentially that first published by Genereaux (1937).

The cost equations can be developed by considering a 1-meter length of pipe.

The purchase cost will be roughly proportional to the diameter raised to some power.

$$\text{Purchase cost} = Bd^n \$/\text{m}$$

The value of the constant B and the index n depend on the pipe material and schedule.

The installed cost can be calculated by using the factorial method of costing discussed in Chapter 7.

$$\text{Installed cost} = Bd^n(1+F)$$

where the factor F includes the cost of valves, fittings, and erection for a typical run of the pipe.

The capital cost can be included in the operating cost as an annual capital charge. There will also be an annual charge for maintenance, based on the capital cost.

$$C_C = Bd^n(1+F)(a+b) \tag{20.25}$$

where C_C = annualized capital cost of the piping, \$/m.yr
a = capital annualization factor, yr^{-1}
b = maintenance costs as fraction of installed capital, yr^{-1}

The power required for pumping is given by:

$$\text{Power} = \text{volumetric flow rate} \times \text{pressure drop}$$

Only the friction pressure drop need be considered, as any static head is not a function of the pipe diameter.

To calculate the pressure drop, the pipe friction factor must be known. This is a function of Reynolds number, which is in turn a function of the pipe diameter. Several expressions have been proposed for relating friction factor to Reynolds number. For simplicity, the relationship proposed by Genereaux (1937) for turbulent flow in clean commercial steel pipes will be used.

$$C_f = 0.04\mathrm{Re}^{-0.16}$$

where C_f is the Fanning friction factor $= 2(R/\rho u^2)$.

Substituting this into the Fanning pressure drop equation gives:

$$\Delta P = 0.125 m^{1.84}\mu^{0.16}\rho^{-1} d_i^{-4.84} \tag{20.26}$$

where ΔP = pressure drop, N/m^2 (Pa)
μ = viscosity, Nm^{-2} s

The annual pumping costs will be given by:

$$C_w = \frac{Ap}{1000\eta}\,\Delta P\,\frac{m}{\rho} \tag{20.27}$$

where A = plant attainment, hours/year
p = cost of power, \$/kWh
η = pump efficiency

Substituting from Equation 20.26:

$$C_w = \frac{Ap}{\eta}\,1.25 \times 10^{-4}\, m^{2.84}\,\mu^{0.16}\,\rho^{-2}\,d_i^{-4.84} \tag{20.28}$$

The total annual operating cost $C_t = C_C + C_w$.

Adding Equations 20.25 and 20.28, differentiating, and equating to zero to find the pipe diameter to give the minimum cost gives:

$$d_i,\ \text{optimum} = \left(\frac{6.05 \times 10^{-4}\, A\, p\, m^{2.84}\,\mu^{0.16}\,\rho^{-2}}{\eta\, n\, B\,(1+F)(a+b)}\right)^{1/(4.84\,+\,n)} \tag{20.29}$$

Equation 20.29 is a general equation and can be used to estimate the economic pipe diameter for any particular situation. It can be set up on a spreadsheet and the effect of the various factors investigated.

The equation can be simplified by substituting typical values for the constants.

- A The normal attainment for a chemical process plant will be between 90% and 95%, so take the operating hours per year as 8000.
- η Pump and compressor efficiencies will be between 50% and 70%, so take 0.6.
- p A typical wholesale cost of electric power for a large user is 0.06 \$/kWh (mid-2011).
- F This is the most difficult factor to estimate. Other authors have used values ranging from 1.5 (Peters & Timmerhaus, 1968) to 6.75 (Nolte, 1978). It is best taken as a function of the pipe diameter, as has been done to derive the simplified equations given later.
- B, n Can be estimated from the current cost of piping.
- a Will depend on the current cost of capital and could range from 0.1 to 0.25, but is typically around 0.16. See Chapter 9 for a detailed discussion.
- b A typical figure for a process plant will be 5%; see Chapter 8.

F, B, and n are best established from a recent correlation of piping costs and should include the costs of fittings, paint or insulation, and installation. The following correlations were derived in January 2006 and can be updated by multiplying by the Chemical Engineering piping cost index, which is published monthly in *Chemical Engineering*. The value of the Chemical Engineering piping index in January 2006 was 655.9, and in January 2010 was 794.5, so the correlations can be updated to a January 2010 basis by multiplying by 794.5/655.9 = 1.21. Note that the cost index is specific to the costs of piping, valves, and fittings and is not the same as the Chemical Engineering plant cost index.

A106 Carbon steel

$$1 \text{ to } 8 \text{ inches}, \$/\text{ft} = 17.4 \left(d_i \text{ in inches}\right)^{0.74}$$

$$10 \text{ to } 24 \text{ inches}, \$/\text{ft} = 1.03 \left(d_i \text{ in inches}\right)^{1.73}$$

304 Stainless steel

$$1 \text{ to } 8 \text{ inches}, \$/\text{ft} = 24.5 \left(d_i \text{ in inches}\right)^{0.9}$$

$$10 \text{ to } 24 \text{ inches}, \$/\text{ft} = 2.74 \left(d_i \text{ in inches}\right)^{1.7}$$

In metric units (d_i in meters), these become:
A106 Carbon steel

$$25 \text{ to } 200 \text{ mm}, \$/\text{m} = 880\ d_i^{0.74}$$

$$250 \text{ to } 600\text{mm}, \$/\text{m} = 1900\ d_i^{1.73}$$

304 Stainless steel

$$25 \text{ to } 200 \text{ mm}, \$/\text{m} = 2200\ d_i^{0.94}$$

$$250 \text{ to } 600\text{mm}, \$/\text{m} = 4700\ d_i^{1.7}$$

For small-diameter carbon steel pipes, substitution in Equation 20.29 gives:

$$d_i, \text{optimum} = 0.830 m^{0.51} \mu^{0.03} \rho^{-0.36}$$

Because the exponent of the viscosity term is small, its value will change very little over a wide range of viscosity

$$\mu = 10^{-5}\ \text{Nm}^{-2}\text{s}\ (0.01\ \text{cp}), \mu^{0.03} = 0.71$$

at

$$\mu = 10^{-2}\ \text{Nm}^{-2}\text{s}\ (10\ \text{cp}), \mu^{0.03} = 0.88$$

Taking a mean value of 0.8 gives the following equations for the optimum diameter for turbulent flow:
A106 Carbon steel pipe:

$$\begin{aligned} 25 \text{ to } 200 \text{ mm}, &\quad d_i, \text{optimum} = 0.664\ m^{0.51}\ \rho^{-0.36} \\ 250 \text{ to } 600 \text{ mm}, &\quad d_i, \text{optimum} = 0.534\ m^{0.43}\ \rho^{-0.30} \end{aligned} \tag{20.30}$$

304 Stainless steel pipe:

$$\begin{aligned} 25 \text{ to } 200 \text{ mm}, &\quad d_i, \text{optimum} = 0.550\ m^{0.49}\ \rho^{-0.35} \\ 250 \text{ to } 600 \text{ mm}, &\quad d_i, \text{optimum} = 0.465\ m^{0.43}\ \rho^{-0.31} \end{aligned} \tag{20.31}$$

Note that the optimum diameter for stainless steel is smaller than for carbon steel, as would be expected given the higher materials cost of the pipe. Note also that Equations 20.30 and 20.31 predict optimum pipe diameters that are roughly double those given by the rule of thumb at the start of this section. This most likely reflects a change in the relative values of capital and energy since the period when the rule of thumb was deduced.

Equations 20.30 and 20.31 can be used to make an approximate estimate of the economic pipe diameter for normal pipe runs. For a more accurate estimate, or if the fluid or pipe run is unusual, the method used to develop Equation 20.29 can be used, taking into account the special features of the particular pipe run.

For very long pipe systems, such as transportation pipelines, the capital costs of the required pumps should also be included. For gases, the capital cost of compression is much more significant and should always be included in the analysis.

Equations for the optimum pipe diameter with laminar flow can be developed by using a suitable equation for pressure drop in the equation for pumping costs.

The approximate equations should not be used for steam, as the quality of steam depends on its pressure, and hence the pressure drop.

Nolte (1978) gives detailed methods for the selection of economic pipe diameters, taking into account all the factors involved. He gives equations for liquids, gases, steam, and two-phase systems. He includes in his method an allowance for the pressure drop due to fittings and valves, which was neglected in the development of Equation 20.26 and by most other authors.

The use of Equations 20.30 and 20.31 are illustrated in Examples 20.10 and 20.11 and the results compared with those obtained by other authors. The older correlations give lower values for the economic pipe diameters, probably due to changes in the relative values of capital and energy. Note, however, that the refining rule of thumb given at the

start of this section gives optimum pipe diameters roughly twice those predicted from Equations 20.30 and 20.31, perhaps reflecting more conservative pipe sizing in that industry.

Example 20.10

Estimate the optimum pipe diameter for a water flow rate of 10 kg/s, at 20 °C. Carbon steel pipe will be used. Density of water 1000 kg/m^3.

Solution

$$d_i, \text{optimum} = 0.664 \times (10)^{0.51} 1000^{-0.36}$$
$$= \underline{177 \text{ mm}} \tag{20.30}$$

177 mm is 6.97 inches, which is not a standard pipe size. We can choose either 6-inch or 8-inch pipe, so try 6-inch pipe, sch 40, inside diameter 6.065 inches (154 mm).

Viscosity of water at 20 °C = 1.1×10^{-3} Ns/m^2,

$$\text{Re} = \frac{4\,m}{\pi\,\mu\,d} = \frac{4 \times 10}{\pi \times 1.1 \times 10^{-3} \times 154 \times 10^{-3}} = 7.51 \times 10^4$$

>4000, so flow is turbulent.

Comparison of methods:

	Economic diameter
Equation 20.30	180 mm
Peters and Timmerhaus (1991)	4 in. (100 mm)
Nolte (1978)	80 mm

Example 20.11

Estimate the optimum pipe diameter for a flow of HCl of 7000 kg/h at 5 bar, 15 °C, stainless steel pipe. Molar volume 22.4 m^3/kmol, at 1 bar, 0 °C.

Solution

Molecular weight HCl = 36.5.

$$\text{Density at operating conditions} = \frac{36.5}{22.4} \times \frac{5}{1} \times \frac{273}{288} = \underline{7.72 \text{ kg/m}^3}$$
$$\text{Optimum diameter} = 0.465 \left(\frac{7000}{3600}\right)^{0.43} \times 7.72^{-0.31} = \underline{328.4 \text{ mm}} \tag{20.31}$$

which is 12.9 inches, so we can use 14-inch pipe, sch 40, with inside diameter 13.124 inch (333 mm).

Viscosity of HCl 0.013 m Ns/m^2

$$\text{Re} = \frac{4}{\pi} \times \frac{7000}{3600} \times \frac{1}{0.013 \times 10^{-3} \times 333 \times 10^{-3}} = \underline{5.71 \times 10^5}, \text{ turbulent}$$

Comparison of methods:

	Economic diameter
Equation 20.31	14 in. (333 mm)
Peters and Timmerhaus (1991)	9 in. (220 mm) carbon steel
Nolte (1978)	7 in. (180 mm) carbon steel

Example 20.12

Calculate the line size and specify the pump required for the line shown in Fig. 20.21: material ortho-dichlorobenzene (ODCB), flow rate 10,000 kg/h, temperature 20 °C, pipe material carbon steel.

Solution

ODCB density at 20 °C = 1306 kg/m^3.
Viscosity: 0.9 mNs/m^2 (0.9 cp).

Estimation of pipe diameter required

typical velocity for liquid 1 m/s

$$\text{mass flow} = \frac{10^4}{3600} = 2.78 \text{ kg/s}$$

$$\text{volumetric flow} = \frac{2.78}{1306} = 2.13 \times 10^{-3} \text{ m}^3/\text{s}$$

$$\text{area of pipe} = \frac{\text{volumetric flow}}{\text{velocity}} = \frac{2.13 \times 10^{-3}}{1} = 2.13 \times 10^{-3} \text{ m}^2$$

$$\text{diameter of pipe} = \sqrt{\left(2.13 \times 10^{-3} \times \frac{4}{\pi}\right)} = 0.052 \text{ m} = 52 \text{ mm}$$

Or use the economic pipe diameter formula:

$$d, \text{optimum} = 0.664 \times 2.78^{0.51} \times 1306^{-0.36}$$
$$= 78.7 \text{ mm} \tag{20.30}$$

Take diameter as 77.9 mm (3-in., sch 40 pipe):

$$\text{cross-sectional area} = \frac{\pi}{4}\left(77.9 \times 10^{-3}\right)^2 = 4.77 \times 10^{-3} \text{ m}^2$$

Pressure drop calculation

$$\text{fluid velocity} = \frac{2.13 \times 10^{-3}}{4.77 \times 10^{-3}} = 0.45 \text{ m/s}$$

Friction loss per unit length, Δf_1:

$$\text{Re} = \frac{1306 \times 0.45 \times 77.9 \times 10^{-3}}{0.9 \times 10^{-3}} = 5.09 \times 10^4 \tag{20.2}$$

Absolute roughness commercial steel pipe, Table 20.3 = 0.46 mm
Relative roughness, $e/d = 0.046/80 = 0.0005$
Friction factor from Fig. 20.5, $f = 0.0025$

$$\Delta f_1 = 8 \times 0.0025 \times \frac{1}{77.9 \times 10^{-3}} \times 1306 \times \frac{0.45^2}{2} = 33.95 \text{ N/m}^2 \tag{20.1}$$

Design for a maximum flow rate of 20% above the average flow:

$$\text{Friction loss} = 0.0339 \times 1.2^2 = 0.0489 \text{ kPa/m}$$

Miscellaneous losses

Take as equivalent pipe diameters. All bends will be taken as 90-degree standard radius elbow.
Line to pump suction:

$$\text{length} = 1.5 \text{ m}$$

$$\text{bend}, 1 \times 30 \times 80 \times 10^{-3} = 2.4 \text{ m}$$

$$\text{valve}, 1 \times 18 \times 80 \times 10^{-3} = 1.4 \text{ m}$$

$$\text{total } 5.3 \text{ m}$$

$$\text{entry loss} = \frac{\rho u^2}{2} \text{(see Section 20.4)}$$

$$\text{at maximum design velocity} = \frac{1306\ (0.45\ \times 1.2)^2}{2\ \times\ 10^3} = 0.19\ \text{kPa}$$

Control valve pressure drop, allow normal 140 kPa

$(\times 1.2^2)$maximum 200 kPa

Heat exchanger, allow normal 70 kPa

$(\times 1.2^2)$maximum 100 kPa

Orifice, allow normal 15 kPa

$(\times 1.2^2)$maximum 22 kPa

Line from pump discharge:

$$\text{length} = 4 \times 5.5 + 20 + 5 + 0.5 + 1 + 6.5 + 2 = 44.5\ \text{m}$$

$$\text{bends}, 6 \times 30 \times 80 \times 10^{-3} = 14.4 = 14.4\ \text{m}$$

$$\text{valves}, 3 \times 18 \times 80 \times 10^{-3} = 4.4 = 4.4\ \text{m}$$

$$63.4\ \text{m}$$

The line pressure-drop calculation is set out on the calculation sheet shown in Table 20.7. A blank version of this calculation sheet can be found online in Appendix G and is also available in Microsoft Excel format at www.elsevier.com/books-and-journals/book-companion/9780128211793.

Pump selection:

$$\text{flow rate} = 2.13 \times 10^{-3} \times 3600 = 7.7\ \text{m}^3/\text{h}$$

$$\text{differential head, maximum}, \underline{\underline{38\ \text{m}}}$$

select single-stage centrifugal (Fig. 20.3)

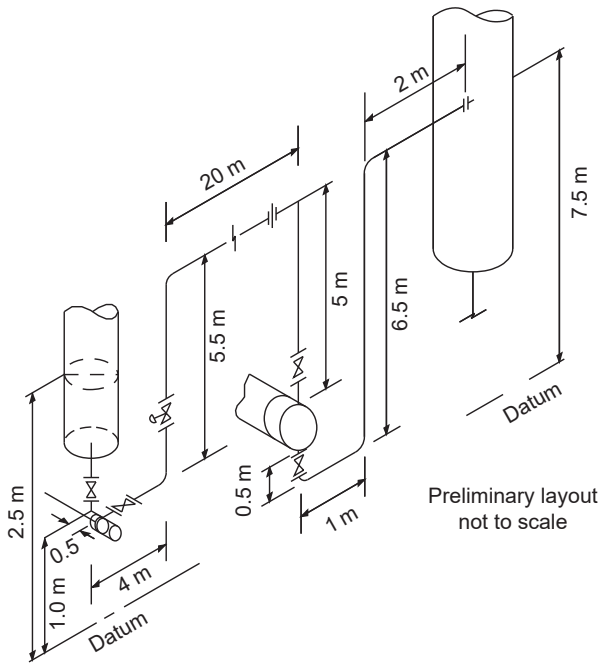


FIG. 20.21 Piping isometric drawing (Example 20.12).

TABLE 20.7 Line calculation form (Example 20.12)

Company Name
Address

Pump and Line Calculation Sheet

Form XXXXX-YY-ZZ

Project Name
Project Number — Sheet 1 of 1

REV	DATE	BY	APVD	REV	DATE	BY	APVD
1	8.7.06	GPT					

Owner's Name
Plant Location
Case Description: Chapter 5 Example 5.4

Equipment label: P101 — Equipment name: Stripper bottoms pump
Plant section
Process service
Fluid: ODCB — Density: 1306 kg/m^3
Operating temperature: Normal 20 °C — Viscosity: 0.9 N.s/m^2
Min 15 °C — Normal flow rate: 2.78 kg/s
Max 30 °C — Design flow rate: 3.34 kg/s

LINE PRESSURE DROP

SUCTION

	Line size		77.9	mm
Note		Normal	Max.	Units
u_1	Velocity	0.4	0.5	m/s
Δf_1	Friction loss	0.03	0.05	kPa/m
L_1	Line length	5.30	5.30	m
$\Delta f_1 L_1$	Line loss	0.18	0.26	kPa
$\rho u_1^2/2$	Entrance loss	0.130	0.188	kPa
(40 kPa)	Strainer			kPa
	(1) Sub-total	0.310	0.446	kPa
z_1	Static head	1.5	1.5	m
$\rho g z_1$		19.2	19.2	kPa
	Upstream equipment pressure	100	100	kPa
	(2) Sub-total	119.2	119.2	kPa
(2) – (1)	(3) Suction pressure	118.9	111.8	kPa
	(4) Vapor pressure	0.1	0.1	kPa
(3) – (4)	(5) NPSH available	118.8	111.7	kPa
(5)/ρg	NPSH available	9.3	8.7	m
	NPSH available	12.1	11.4	m water

DISCHARGE

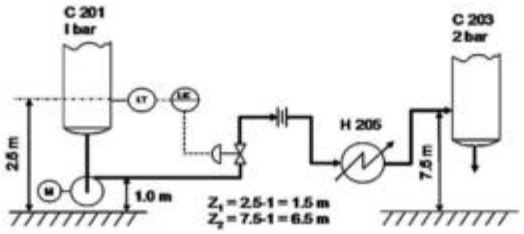
	Line size		77.9	mm
Note	Flow	Normal	Max.	Units
u_2	Velocity	0.4	0.5	m/s
Δf_2	Friction loss	0.03	0.05	kPa/m
L_2	Line length	63.4	63.4	m
$\Delta f_2 L_2$	Line loss	2.15	3.09	kPa
	Orifice / Flow meter	15	22	kPa
	Control valve	140	200	kPa
	Equipment			
S&THX	H 205	70	100	kPa
				kPa
				kPa
Total	(6) Dynamic loss	227	325	kPa
z_2	Static head	6.5	6.5	m
$\rho g z_2$		83.3	83.3	kPa
	Equip. press (max)	200	200	kPa
	Contingency	0	0	kPa
	(7) Sub-total	283.3	283.3	kPa
(7) + (6)	Discharge pressure	510.4	608.4	kPa
(3)	Suction pressure	118.9	111.8	kPa
	(8) Differential pressure	391.5	496.6	kPa
(8)/ρg	Pump head	30.6	38.8	m
	Control valve			
Valve/(6)	% Dyn. loss		62%	

PUMP DATA

Pump manufacturer
Catalog No.
Pump flow rate: normal 7.7 m^3/h — max. 9.2 m^3/h
Differential pressure: 391.5 kPa; 30.6 m; 39.9 m water
NPSH required: m
Pump type
No. of stages: single
Impeller type: closed
Mounting: horizontal

Driver type: Electric 3-phase
Power supply: 440 V
Seal type: Mechanical, external flush
Hydraulic power: 0.833 kW
Rated power: kW
Efficiency: %
Suction specific speed
Casing design pressure: 610 kPa
Casing design temperature: 30 °C
Casing type
Casing material

SKETCH



NOTES

1. Process data completed, remaining information to be filled in after equipment selection
2.
3.
4.
5.

20.11 Sizing of control valves

The pressure drop required across a control valve will be a function of the valve, pump, and piping design and will set the size of valve that is selected. Sufficient pressure drop must be allowed for when sizing the pump, valve, and piping system to ensure that the control valve operates satisfactorily over the full range of flow required. If possible, the control valve and pump should be sized together, as a unit, to ensure that the optimum size is selected for both.

All control valves operate by manipulating a resistance to flow and hence controlling a flow rate, regardless of the function of the control loop. The signal from the valve actuator causes a variation in the size of a restriction in the fluid flow path, leading to an increase or decrease in fluid flow.

Most automatic control valves are globe valves, although butterfly valves are sometimes used for gases and vapors, and diaphragm valves and ball valves are occasionally used. Illustrations of the different types of valves are given in Section 20.5. A plug-disk—type globe valve has several contributions to fluid pressure drop. As the fluid enters the valve, it makes a sharp 90-degree turn, enters an area of expanded cross-section below the valve seat, passes through the variable annular space between the disk and the seat of the valve into the space above the disk, and then makes another sharp 90-degree turn to leave the valve. As the valve opens, the annular space increases and the pressure drop across the valve falls, but even in the fully open position there is still a substantial pressure drop across the valve. The pressure drop across the valve varies between about 9 velocity heads in the fully open position and about 112 velocity heads when one-quarter open, depending on the valve design (see Table 20.4). The system pressure drop curves for both the fully open and 25% open cases (or minimum percent open recommended by the valve manufacturer) can be plotted against the pump curve to determine the controllable range of flow rate for the proposed pump and piping system, as described in Section 20.7.5.

As a rough guide, if the characteristics are not specified, the control valve pressure drop should be taken as at least 30% of the total dynamic pressure drop through the system, with a minimum value of 100 kPa (14 psi). A good rule of thumb in the early stages of process design is to allow 140 kPa (20 psi) pressure drop for each control valve if the pressure drop in the process equipment is not yet known. Some of the pressure drop across the valve will be recovered downstream, with the amount depending on the type of valve used.

Detailed methods for control valve sizing are given in the ISA S75.01 standard and have been implemented in computer design tools that are used by instrument engineers and valve manufacturers. The detailed methods can account for choked flow, compressible flow, laminar flow, flashing liquids, and cavitation.

For nonchoked, turbulent flow of an incompressible fluid, ISA 75.01.01-2007 gives the following equation for valve sizing:

$$C_v = \frac{Q}{N}\sqrt{\frac{\rho_1/\rho_0}{\Delta P}} \tag{20.32}$$

where C_v = valve flow coefficient
Q = volumetric flow
ρ_1 = fluid density at flow conditions
ρ_0 = density of water at 15 °C, i.e., ρ_1/ρ_0 = fluid specific gravity
N = a constant, depending on the units used (see later)
ΔP = pressure drop = $P_1 - P_2$, where:
P_1 = pressure measured two nominal pipe diameters upstream of the valve
P_2 = pressure measured six nominal pipe diameters downstream of the valve

The value of the constant N depends on the units used. If the volumetric flow rate is given in gallons per minute and the pressure drop in pounds per square inch, then $N = 1$, so the valve coefficient can be interpreted as the flow rate of water in gpm that will flow through the valve with 1 psi pressure drop at 15 °C (59 °F). If the flow rate is given in m^3/h and the pressure drop in bar, then $N = 0.865$.

Different formulae are given for C_v for compressible fluids, choked flow, laminar flow, and other conditions in the ISA S75.01 standard.

Control valves should always be sized for a flow rate larger than the normal flow condition. Different companies use different methods for determining how much design margin to incorporate in control valve sizing. A simple method is to calculate C_v based on the normal flow rate and then select a valve that has twice this value of C_v, so that in normal operation the valve will be roughly 50% open. Another popular method is to calculate C_v based

on a maximum flow rate 30% above the normal stream flow rate, then divide the result by 0.7 and pick the valve with the next largest C_v. This gives a valve with C_v equal to 1.85 times the value calculated for normal flow, which in normal operation will be about 54% open.

The ratio between the maximum and minimum controllable flow rates is known as the *rangeability* of the valve. The installed rangeability is influenced by the actuator and positioner, as well as the valve design. The ratio of the normal maximum flow to the minimum controllable flow is called the *turndown* of the valve. For most control valves, the turndown is about 70% of the rangeability. Rangeability typically varies between about 20 and 50. The designer should consider the desired turndown and rangeability when selecting valves, particularly in level control applications where the process may call for a high range of operable flow rates. When high rangeability is required, two control valves of different sizes with slightly overlapping operating ranges can be used in parallel. This is known as a *split-range* arrangement. Control valve characteristics and rangeability are discussed in more detail in the ISA S75.11 standard.

Example 20.13

The feed media to a fermentation reactor consists of glucose solution in water with added nutrients and has specific gravity 1.03 at 40 °C. Determine the size of control valve to use for a normal design flow rate of 0.2 m^3/h if the valve is sized with a pressure drop of 1.25 bar.

Solution

For metric units, $N = 0.865$ in Equation 20.32, so for normal flow conditions:

$$C_v = \frac{0.2}{0.865}\sqrt{\frac{1.03}{1.25}} = 0.210 \tag{20.32}$$

Select a valve that has $C_v \approx 0.42$ so that valve normally operates about 50% open.

20.12 References

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20.13 Nomenclature

		Dimensions in MLT$
A	Plant attainment (hours operated per year)	—
B	Purchased cost factor, pipes	$\mathbf{\$L^{-1}}$
a	Capital charges factor, piping	$\mathbf{T^{-1}}$
b	Maintenance cost factor, piping	$\mathbf{T^{-1}}$
C	Sum of mechanical, corrosion and erosion allowances	$\mathbf{L}$
C_f	Fanning friction factor	—
C_C	Annual capital charge, piping	$\mathbf{\$L^{-1}T^{-1}}$
C_p	Specific heat at constant pressure	$\mathbf{L^2T^{-2}\theta^{-1}}$
C_t	Total annual cost, piping	$\mathbf{\$L^{-1}T^{-1}}$
$C\upsilon$	Specific heat at constant volume	$\mathbf{L^2T^{-2}\theta^{-1}}$
$C\upsilon$	Control valve sizing parameter (Equation 20.32)	—
C_w	Annual pumping cost, piping	$\mathbf{\$L^{-1}T^{-1}}$
d	Pipe diameter	$\mathbf{L}$
d_i	Pipe inside diameter	$\mathbf{L}$
E	Pipe casting quality factor	—
E_e	Efficiency, electric motors	—
E_p	Polytropic efficiency, compressors, and turbines	—
e	Relative roughness	—
F	Installed cost factor, piping	—
f	Friction factor	—
g	Gravitational acceleration	$\mathbf{LT^{-2}}$
H	Enthalpy (Equation 20.8)	$\mathbf{ML^2T^{-2}}$
H	Height of liquid above the pump suction	$\mathbf{L}$
h	Pump head	$\mathbf{L}$
K	Number of velocity heads	—
L	Pipe length	$\mathbf{L}$
M_w	Molecular mass (weight)	—
m	Polytropic temperature exponent	—
m	Mass flow rate	$\mathbf{MT^{-1}}$
N	Pump speed, revolutions per unit time	$\mathbf{T^{-1}}$
N	Control valve constant (Equation 20.32)	—
N_s	Pump specific speed	—
n	Index relating pipe cost to diameter	—
P	Pressure	$\mathbf{ML^{-1}T^{-2}}$
P_c	Critical pressure	$\mathbf{ML^{-1}T^{-2}}$
P_F	Pressure loss in suction piping	$\mathbf{ML^{-1}T^{-2}}$
P_i	Interstage pressure	$\mathbf{ML^{-1}T^{-2}}$

(continued)

		Dimensions in MLT$
P_r	Reduced pressure	—
P_s	Safe working pressure	$\mathbf{ML^{-1}T^{-2}}$
P_v	Vapor pressure of liquid	$\mathbf{ML^{-1}T^{-2}}$
P_1	Initial pressure	$\mathbf{ML^{-1}T^{-2}}$
P_2	Final pressure	$\mathbf{ML^{-1}\ T^{-2}}$
ΔP	Difference in system pressures ($P_1 - P_2$)	$\mathbf{ML^{-1}T^{-2}}$
ΔP_f	Pressure drop due to friction	$\mathbf{ML^{-1}T^{-2}}$
p	Cost of power, pumping	$\mathbf{\$M^{-1}L^{-2}T^{2}}$
Q	Volumetric flow rate	$\mathbf{L^{3}T^{-1}}$
R	Shear stress on surface, pipes	$\mathbf{ML^{-1}T^{-2}}$
R	Universal gas constant	$\mathbf{L^{2}T^{-2}\theta^{-1}}$
S	Basic allowable stress for pipe material	$\mathbf{ML^{-1}T^{-2}}$
T	Temperature, absolute	$\boldsymbol{\theta}$
T_c	Critical temperature	$\boldsymbol{\theta}$
T_r	Reduced temperature	—
T_1	Initial temperature	$\boldsymbol{\theta}$
T_2	Final temperature	$\boldsymbol{\theta}$
t	Pipe wall thickness	**L**
t_m	Minimum required thickness	**L**
t_p	Pressure design thickness	**L**
u	Fluid velocity	$\mathbf{LT^{-1}}$
v	Volume per unit mass	$\mathbf{M^{-1}L^{3}}$
W	Work done	$\mathbf{L^{2}T^{-2}}$
Z	Compressibility factor	—
z	Height above datum	**L**
Δz	Difference in elevation ($z_1 - z_2$)	**L**
γ	Ratio of specific heats	—
γ_T	Temperature coefficient	—
η	Pump efficiency	—
η_t	Turbine efficiency	—
ρ	Fluid density	$\mathbf{ML^{-3}}$
ρ_0	Density of water at 15 °C	$\mathbf{ML^{-3}}$
ρ_1	Fluid density of flowing fluid at process conditions	$\mathbf{ML^{-3}}$
μ	Viscosity of fluid	$\mathbf{ML^{-1}T^{-1}}$
σ_d	Design stress	$\mathbf{ML^{-1}T^{-2}}$
σ_s	Safe working stress	$\mathbf{ML^{-1}T^{-2}}$
Re	Reynolds number	—
$NPSH_{avail}$	Net positive suction head available at the pump suction	**L**
$NPSH_{reqd}$	Net positive suction head required at the pump suction	**L**

20.14 Problems

20.1. Select suitable valve types for the following applications:

1. Isolating a heat exchanger.
2. Manual control of the water flow into a tank used for making up batches of sodium hydroxide solution.
3. The valves need to isolate a pump and provide emergency manual control on a bypass loop.
4. Isolation valves in the line from a vacuum column to the steam ejectors producing the vacuum.
5. Valves in a line where cleanliness and hygiene are an essential requirement.
State the criterion used in the selection for each application.

20.2 A supply of nitrogen is required as an inert gas for blanketing and purging vessels. After generation, the nitrogen is compressed and stored in a bank of cylinders at a pressure of 5 barg. The inlet pressure to the compressor is 0.5 barg, and the temperature is 20 °C. Calculate the maximum power required to compress 100 m^3/h. A single-stage reciprocating compressor will be used.

20.3. Hydrogen chloride gas, produced by burning chlorine with hydrogen, is required at a supply pressure of 600 kN/m^2 gauge. The pressure can be achieved by either operating the burner under pressure or by compressing the hydrogen chloride gas. For a production rate of hydrogen chloride of 10,000 kg/h, compare the power requirement of compressing the hydrogen supply to the burner with that to compress the product hydrogen chloride. The chlorine feed is supplied at the required pressure from a vaporizer. Both the hydrogen and chlorine feeds are essentially pure. Hydrogen is supplied to the burner in 1% excess of the stoichiometric requirement.
A two-stage centrifugal compressor will be used for both duties. Take the polytropic efficiency for both compressors as 70%. The hydrogen supply pressure is 120 kN/m^2 and the temperature 25 °C. The hydrogen chloride is cooled to 50 °C after leaving the burner. Assume that the compressor intercooler cools the gas to 50 °C for both duties.
Which process would you select and why?

20.4. Estimate the work required to compress ethylene from 32 MPa to 250 MPa in a two-stage reciprocating compressor where the gas is initially at 30 °C and leaves the intercooler at 30 °C.

20.5. Crude dichlorobenzene is pumped from a storage tank to a distillation column.
The tank is blanketed with nitrogen, and the pressure above the liquid surface is held constant at 0.1 bar gauge pressure. The minimum depth of liquid in the tank is 1 m.
The distillation column operates at a pressure of 500 mmHg (500 mm of mercury, absolute). The feed point to the column is 12 m above the base of the tank. The tank and column are connected by a 50 mm internal diameter commercial steel pipe, 200 m long. The pipe run from the tank to the column contains the following valves and fittings: 20 standard radius 90-degree elbows; two gate valves to isolate the pump (operated fully open); an orifice plate and a flow-control valve.
If the maximum flow rate required is 20,000 kg/h, calculate the pump motor rating (power) needed. Take the pump efficiency as 70% and allow for a pressure drop of 0.5 bar across the control valve and a loss of 10 velocity heads across the orifice. Density of dichlorobenzene 1300 kg/m^3, viscosity 1.4 cp.

20.6. A liquid is contained in a reactor vessel at 115 bar absolute pressure. It is transferred to a storage vessel through a 50 mm internal diameter commercial steel pipe. The storage vessel is nitrogen blanketed, and pressure above the liquid surface is kept constant at 1500 N/m^2 gauge. The total run of pipe between the two vessels is 200 m. The miscellaneous losses due to entry and exit losses, fittings, valves, etc., amount to 800 equivalent pipe diameters. The liquid level in the storage vessel is at an elevation 20 m *below* the level in the reactor.
A turbine is fitted in the pipeline to recover the excess energy that is available over that required to transfer the liquid from one vessel to the other. Estimate the power that can be taken from the turbine when the liquid transfer rate is 5000 kg/h. Take the efficiency of the turbine as 70%.
The properties of the fluid are density 895 kg/m^3, viscosity 0.76 $mNm^{-2}s$.

20.7. A process fluid is pumped from the bottom of one distillation column to another using a centrifugal pump. The line is standard commercial steel pipe 75 mm internal diameter. From the column to the pump inlet,

the line is 25 m long and contains six standard elbows and a fully open gate valve. From the pump outlet to the second column, the line is 250 m long and contains 10 standard elbows, four gate valves (operated fully open), and a flow-control valve. The fluid level in the first column is 4 m above the pump inlet. The feed point of the second column is 6 m above the pump inlet. The operating pressure in the first column is 1.05 bara and that of the second column 0.3 barg.
Determine the operating point on the pump characteristic curve when the flow is such that the pressure drop across the control valve is 35 kN/m^2. The physical properties of the fluid are density 875 kg/m^3, viscosity 1.46 mN m^{-2}s.
Also, determine the NPSH at this flow rate if the vapor pressure of the fluid at the pump suction is 25 kN/m^2.
Pump characteristics:

Flow rate, m^3/h	0.0	18.2	27.3	36.3	45.4	54.5	63.6
Head, m of liquid	32.0	31.4	30.8	29.0	26.5	23.2	18.3

20.8. Revisiting Example 20.8, suppose the flow was controlled using a plug-disk globe valve and the initial design in the example assumed that the valve is fully open. What range of flow rates can be achieved if the valve can be throttled down to quarter open? When the valve is quarter open, what fraction of the pump work is lost across the valve?

20.9. Estimate the shaft work required to pump 65 gal/min of sugar solution in water (specific gravity = 1.05) if the pump inlet pressure is 25 psig and the outlet pressure required is 155 psig.

20.10 A shell and tube cooler in an aromatics complex cools 26,200 lb/h of naphtha (specific gravity 0.78, viscosity 0.007 cP). The cooler has 347 tubes, 16 ft long, ¾-inch diameter. If the naphtha is on the tube side, estimate the tube side pressure drop.

20.11 In a detergent-making process, 1400 gal/h of water flows through a 2-inch pipe system as follows:
Exit from pump, 2 ft vertical, open gate valve, 14 ft vertical, 90-degree bend, 12 ft horizontal, quarter open globe valve, 20 ft horizontal, 90-degree bend, 6 ft horizontal, 90-degree bend, 12 ft vertical, 90-degree bend, 14 ft horizontal, 90-degree bend, 4 ft vertical, 90-degree bend, 28 ft horizontal, open gate valve, 3 ft horizontal, entry to tank containing 30 ft of liquid.

a. If the pump and tank are both at grade level, estimate the head that the pump must deliver.
b. If the pump inlet pressure is 25 psig, what is the outlet pressure?
c. Estimate the pump shaft work.
d. If the pump is powered by an electric motor with 85% efficiency, what is the annual electricity consumption?

20.12 What size control valve would you select to regulate a flow of 4 m^3/h of liquid of specific gravity 0.7 if the desired valve pressure drop is 140 kPa?

Appendices

APPENDIX A: GRAPHICAL SYMBOLS FOR PIPING SYSTEMS AND PLANT

Available at http://www.elsevier.com/books-and-journals/book-companion/9780128211793.

APPENDIX B: CORROSION CHARTS

Available at http://www.elsevier.com/books-and-journals/book-companion/9780128211793.

APPENDIX C: PHYSICAL PROPERTY DATA BANK

Available at http://www.elsevier.com/books-and-journals/book-companion/9780128211793.

APPENDIX D: CONVERSION FACTORS

An asterisk (*) denotes an exact relationship			
Length	*1 in.	:	25.4 mm
	*1 ft	:	0.3048 m
	*1 yd	:	0.9144 m
	1 mile	:	1.6093 km
	*1 Å (angstrom)	:	10^{-10} m
Time	*1 min	:	60 s
	*1 h	:	3.6 ks
	*1 day	:	86.4 ks
	1 year	:	31.5 Ms
Area	*1 $in.^2$	:	645.16 mm^2
	1 ft^2	:	0.092903 m^2
	1 yd^2	:	0.83613 m^2
	1 acre	:	4046.9 m^2
	1 $mile^2$	:	2.590 km^2
Volume	1 $in.^3$	:	16.387 cm^3
	1 ft^3	:	0.02832 m^3
	1 yd^3	:	0.76453 m^3

(*Continued*)

An asterisk (*) denotes an exact relationship—Cont'd			
	1 UK gal	:	4546.1 cm^3
	1 US gal	:	3785.4 cm^3
	1 short (US) ton	:	907.18 kg
Mass	1 oz	:	28.352 g
	*1 lb	:	0.45359237 kg
	1 cwt	:	50.8023 kg
	1 long (UK) ton	:	1016.06 kg
	1 short (US) ton	:	907.18 kg
Force	1 pdl	:	0.13826 N
	1 lbf	:	4.4482 N
	1 kgf	:	9.8067 N
	1 tonf	:	9.9640 kN
	*1 dyn	:	10^{-5} N
Temperature difference	*1 deg F (deg R)	:	5/9 deg C (deg K)
Energy (work, heat)	1 ft lbf	:	1.3558 J
	1 ft pdl	:	0.04214 J
	*1 cal (internat. table)	:	4.1868 J
	1 erg	:	10^{-7}J
	1 Btu	:	1.05506 kJ
	1 hp h	:	2.6845 MJ
	*1 kW h	:	3.6 MJ
	1 therm	:	105.51 MJ
	1 thermie	:	4.1855 MJ
Calorific value (volumetric)	1 Btu/ft^3	:	37.259 kJ/m^3
Velocity	1 ft/s	:	0.3048 m/s
	1 mile/h	:	0.44704 m/s
Volumetric flow	1 ft^3/s	:	0.028316 m^3/s
	1 ft^3/h	:	7.8658 cm^3/s
	1 UK gal/h	:	1.2628 cm^3/s
	1 US gal/h	:	1.0515 cm^3/s
Mass flow	1 lb/h	:	0.12600 g/s
	1 ton/h	:	0.28224 kg/s
Mass per unit area	1 lb/$in.^2$	:	703.07 kg/m^2
	1 lb/ft^2	:	4.8824 kg/m^2
	1 ton/sq mile	:	392.30 kg/km^2
Density	1 lb/in^3	:	27.680 g/cm^3
	1 lb/ft^3	:	16.019 kg/m^3
	1 lb/UK gal	:	99.776 kg/m^3
	1 lb/US gal	:	119.83 kg/m^3

(*Continued*)

An asterisk (*) denotes an exact relationship—Cont'd			
Pressure	1 lbf/in.^{2} (1 psi)	:	6.8948 kN/m^2
	1 ksi (1000 psi)	:	6.8948 MN/m^2
	1 tonf/in.^{2}	:	15.444 MN/m^2
	1 lbf/ft^2	:	47.880 N/m^2
	*1 standard atm	:	101.325 kN/m^2
	*1 atm (1 kgf/cm^2)	:	98.0665 kN/m^2
	*1 bar	:	10^5 N/m^2
	1 ft water	:	2.9891 kN/m^2
	1 in. water	:	249.09 N/m^2
	1 in. Hg	:	3.3864 kN/m^2
	1 mmHg (1 torr)	:	133.32 N/m^2
Power (heat flow)	1 hp (British)	:	745.70 W
	1 hp (metric)	:	735.50 W
	1 erg/s	:	10^{-7} W
	1 ft lbf/s	:	1.3558 W
	1 Btu/h	:	0.29307 W
	1 ton of refrigeration	:	3516.9 W
Moment of inertia	1 lb ft^2	:	0.042140 kg m^2
Momentum	1 lb ft/s	:	0.13826 kg m/s
Angular momentum	1 lb ft^2/s	:	0.042140 kg m^2/s
Viscosity, dynamic	*1 P (Poise)	:	0.1 N s/m^2
	1 lb/ft h	:	0.41338 mN s/m^2
	1 lb/ft s	:	1.4882 N s/m^2
Viscosity, kinematic	*1 S (Stokes)	:	10^{-4} m^2/s
	1 ft^2/h	:	0.25806 cm^2/s
Surface energy	1 erg/cm^2	:	10^{-3} J/m^2
(surface tension)	(1 dyn/cm)	:	(10^{-3} N/m)
Mass flux density	1 lb/h ft^2	:	1.3562 g/s m^2
Heat flux density	1 Btu/h ft^2	:	3.1546 W/m^2
	*1 kcal/h m^2	:	1.163 W/m^2
Heat transfer coefficient	1 Btu/h ft^2 F	:	5.6783 W/m^2 K
Specific enthalpy (latent heat, etc.)	*1 Btu/lb	:	2.326 kJ/kg
Specific heat capacity	*1 Btu/lb °F	:	4.1868 kJ/kg K
Thermal	1 Btu/h ft °F	:	1.7307 W/m K
conductivity	1 kcal/h m °C	:	1.163 W/m K

Note: Where temperature difference is involved K = °C.
Taken from Mullin, J. W.: The Chemical Engineer *No. 211 (Sept. 1967), 176. SI units in chemical engineering.*

APPENDIX E: DESIGN PROJECTS (SHORTER PROBLEM STATEMENTS)

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Projects include: acetaminophen, acetic acid, acetophenone, acrolein, acrylic acid, alendronate, amlodipine besylate (Norvasc™), ammonia, argon recovery, aspartame, aspirin, benzene reduction, biopulping, black liquor recovery, bromine, carbon nanotubes, cellulose acetate, chemi-mechanical pulping, chlor-alkali, chlorine-free pulp bleaching, chloroform, ciprofloxacin, citalopram hydrobromide (Celexa™), 3-R citronellol, Cleve's acid, clopidogrel (Plavix™), cocoa processing, crude oil distillation, cyclohexanone with phenol, cyclosporin A, dextrins, dicalcium phosphate, dicyclopentadiene, 2,6-dimethyl naphthalene, doxycyline, erythorbic acid, ethanol by fermentation, ethylene by oxidative dehydrogenation, ethylene by steam cracking, ethylene from ethanol, fexofenadine (Allegra™), Fischer-Tropsch catalyst, fluconazole, fluoxetine hydrochloride, fluticasone propionate (Flovent™), folic acid, fuel processor, gas to liquids by Fischer-Tropsch synthesis, granulocyte colony stimulating factor, guaifenesin (Actifed™, Robitussin™), hydrocracking, hydrogen by steam reforming of methane, hydrogen for fuel cells, ibuprofen (Advil™, Motrin™), insect repellant, isomerization of naphtha, Kraft pulping, krypton recovery, lactic acid by fermentation, lansoprazole (Prevacid™), linear alkylbenzenes, lisinopril, loratidine, low-fat snacks, d-malic acid, mannitol, margarine, methanol to olefins, methylene chloride, moisturizing lotion, monosodium glutamate, 2,6-naphthalene dicarboxylic acid, natural gas liquefaction, natural gas liquids recovery, niacinamide, nitric acid, nitrobenzene, s-ofloxacin, omepra-zole (Prilosec™), oxygen (small scale portable/medical), paroxetine (Paxil™), phenol, phosgene, phosphoric acid, polylactic acid, potassium permanganate, propylene by catalytic dehydrogenation, propylene by steam cracking, propylene glycol by fermentation, propylene oxide, pseudoephedrine, pyridine, riboflavin, risperidone (Risperdal), salicylic acid USP, setraline hydrochloride (Zoloft™), simvastatin (Zocor™), sulfur dioxide treatment, sulfur recovery, sumatriptan (Imigran™), tocopherol, toxic waste disposal, urea DSM process, venlafaxine (Effexor™), xenon recovery & zeolite synthesis.

APPENDIX F: DESIGN PROJECTS (LONGER PROBLEM STATEMENTS)

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Projects include: 2-ethylhexanol, acrylonitrile, aniline, chlorine (from hydrogen chloride), chloro-benzenes, hydrogen from fuel oil, methyl ethyl ketone & urea.

APPENDIX G: EQUIPMENT SPECIFICATION (DATA) SHEETS

Available at http://www.elsevier.com/books-and-journals/book-companion/9780128211793.

APPENDIX H: TYPICAL SHELL AND TUBE HEAT EXCHANGER TUBE-SHEET LAYOUTS

Available at http://www.elsevier.com/books-and-journals/book-companion/9780128211793.

APPENDIX I: MATERIAL SAFETY DATA SHEET

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