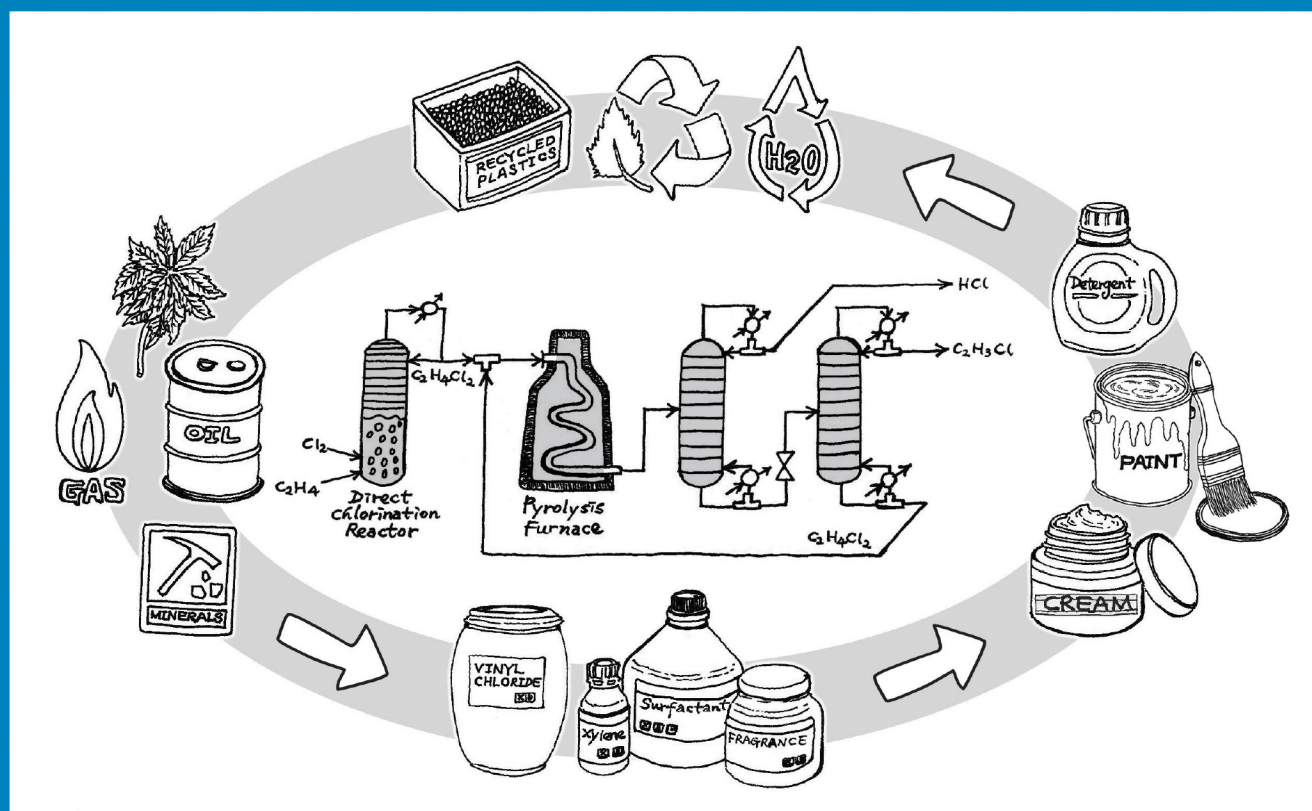


PRODUCT AND PROCESS DESIGN PRINCIPLES

Synthesis, Analysis and Evaluation

FOURTH EDITION



WARREN D. SEIDER • DANIEL R. LEWIN
J.D. SEADER • SOEMANTRI WIDAGDO
RAFIQUL GANI • KA MING NG

WILEY

**PRODUCT AND PROCESS
DESIGN PRINCIPLES**

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Synthesis, Analysis, and Evaluation

Fourth Edition

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Dedication

To the memory of my parents, to Diane, and to Deborah, Gabriel, Joe, Yishai, and Idana; Benjamin, Jaime, Ezra, and Raz

To the memory of my father, Harry Lewin, to my mother, Rebeca Lewin, to Ruti, and to Noa and Yonatan

To the memory of my parents, to Sylvia, and to my children

To the memory of my father, Theodorus Widagdo, to my mother, and to Richard

To the memory of L. E. (Skip) Scriven, H. Ted Davis, and Alkis Payatakes

To the memory of Richard R. Hughes, a pioneer in computer-aided simulation and optimization with whom two of the authors developed many concepts for carrying out and teaching process design

To all of our students: past, present, and future...

About the Authors

Warren D. Seider is Professor of Chemical and Biomolecular Engineering at the University of Pennsylvania. He received a B.S. degree from the Polytechnic Institute of Brooklyn and M.S. and Ph.D. degrees from the University of Michigan. He has contributed to the fields of process analysis, simulation, design, and control. Seider coauthored *FLOWTRAN Simulation—An Introduction* in 1974 and has coordinated the design course involving projects provided by many practicing engineers in the Philadelphia area at Penn for over 35 years. He has authored or coauthored 120 journal articles and authored or edited seven books. Seider was the recipient of the American Institute of Chemical Engineers (AIChE) Computing in Chemical Engineering Award in 1992, corecipient of the AIChE Warren K. Lewis Award in 2004 with J. D. Seader, and recipient of the AIChE F. J. and Dorothy Van Antwerpen Award in 2011. Seider served as Director of AIChE from 1984 to 1986 and as Chairman of the CAST Division and the Publication Committee. He helped to organize the Computer Aids for Chemical Engineering Education (CACHE) Committee in 1969 and served as its chairman. Seider is a member of the Editorial Advisory Board of *Computers and Chemical Engineering*. In 2008, his textbook, *Introduction to Chemical Engineering and Computer Calculations* with coauthor Alan L. Myers, was cited as one of 30 ground-breaking books in the last 100 years of chemical engineering.

Daniel R. Lewin is Churchill Family Chair Professor of Chemical Engineering and Director of the Process Systems Engineering (PSE) research group at the Technion, the Israel Institute of Technology. He received his B.Sc. from the University of Edinburgh and his D.Sc. from the Technion. Lewin's research focuses on the interaction of process design and process control and operations with emphasis on model-based methods. He has authored or coauthored over 100 technical publications in the area of process systems engineering as well as the first three editions of this textbook and the multimedia CD that accompanies it. Lewin has been awarded a number of prizes for research excellence and twice received the Jacknow Award, the Alfred and Yehuda Weissman Award, and the Yannai Prize, in recognition of teaching excellence at the Technion.

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Rafiqul Gani is Professor of System Design at the Department of Chemical & Biochemical Engineering, The Technical University of Denmark. He is also the cofounder and former Head of the Computer Aided Product-Process Engineering Center (CAPEC). He received a B.S. degree from the Bangladesh University of Engineering and Technology, and M.S., DIC, and Ph.D. degrees from Imperial College, London. Gani's current research interests include development of computer-aided methods and tools for modeling, property estimation, process-product synthesis and design, and process-tools integration. He has published more than 300 peer-reviewed journal articles and delivered over 300 lectures, seminars, and plenary/keynote lectures at international conferences, institutions, and companies all over the world. Gani was Editor-in-chief of the *Computers & Chemical Engineering* journal (until 31 December 2015), is Editor of the Elsevier CACE book series, and serves on the editorial advisory board of several other journals. He received the 2015 Computers and Chemical Engineering Award from the AIChE CAST Division. For the term 2016–2017, he has been relected as the President of the European Federation of Chemical Engineering (EFCE); he is a member of the Board of Trustees of the American Institute of Chemical Engineers (AIChE); a Fellow of the AIChE; and a Fellow of Institution of Chemical Engineers (IChemE).

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Preface

OBJECTIVES

The principal objective of this textbook, e-book, and accompanying materials, referred to here as *courseware*, is to present modern strategies for the systematic design of chemical products and processes. Product design deals with “What to Make,” and process design deals with “How to Make.”

Since the early 1960s, undergraduate education of chemical engineers has focused mainly on the engineering sciences. In recent years, however, more scientific approaches to product and process design have been developed, and the need to teach students these approaches has become widely recognized. Consequently, this courseware has been developed to help students and practitioners better use the modern approaches to product and process design. Like workers in thermodynamics; momentum, heat, and mass transfer; and chemical reaction engineering, product and process designers apply the principles of mathematics, chemistry, physics, and biology. Designers also use these principles and those established by engineering scientists to create chemical products and processes that satisfy societal needs while returning a profit. In so doing, designers emphasize the methods of synthesis and optimization in the face of uncertainties, often utilizing the results of analysis and experimentation prepared in cooperation with engineering scientists while working closely with their business colleagues.

This courseware describes the latest design strategies, most of which have been improved significantly by the advent of computers, numerical mathematical programming methods, and artificial intelligence. Because few curricula emphasize design strategies prior to design courses, this courseware is intended to provide a smooth transition for students and engineers who are called upon to design creative new products and processes.

This new edition is a result of an evolution in our approach to teaching design, starting from the first edition, which focused on commodity chemical processes; it was followed by the second edition, which expanded the scope to include the design of chemical products with emphasis on specialty chemicals involving batch rather than continuous processing. This was followed by the third edition, which presented a unified view of the design of basic, industrial, and configured consumer chemical products in the perspective of the Stage-Gate™ Product-Development Process (SGPDP). In this fourth edition, we have organized the presentation of product and process design into two separate, although related, activities in a manner so that the two topics can be taught separately or together. Thus, the reader of this edition can choose to focus only on process design or on product design or can choose to study the two in parallel.

This courseware is intended for seniors and graduate students, most of whom have solved a few open-ended problems but have not received instruction in a systematic approach to product and process design. To guide this instruction, the subject matter is presented in five parts. Part I provides introductions to product design in Chapter 1 and to process design in Chapter 2. The two introductions are then followed by Chapter 3, which provides supporting materials for design activity covering literature sources, energy sources, sustainability and environmental protection, safety, and engineering ethics.

Following the introductions in Part I, Part II deals with the synthesis of products and processes. The first two chapters of this part focus on synthesis issues concerning product design, beginning with the design of molecules and mixtures to satisfy customer needs in Chapter 4. More specifically, Chapter 4 describes the use of computer-aided techniques to identify chemicals (e.g., refrigerants, solvents, polymers) and blends and solvent-based products (e.g., paints, lotions, creams) having desired properties. Chapter 5 focuses on the design of devices, functional products, and formulated products whose structure, form, shape, and/or configuration is customized.

The remainder of Part II provides a sequence of six chapters for a systematic approach to process design, starting with Chapter 6, which shows how heuristics can be harnessed to rapidly generate an initial base-case design without doing much analysis. Next, Chapter 7 presents the computational background to the use of simulation in process design, thus providing a means for verifying the heuristic decisions with quantitative analysis. In this regard, Chapter 7 also presents short-cut computation methods. It includes reliable estimation methods for thermophysical and transport properties. These two chapters are followed by chapters covering the synthesis of reactor networks (Chapter 8) and separation trains (Chapter 9), second-law analysis (Chapter 10), and heat and power integration methodology (Chapter 11). Part II also includes coverage of equipment design: Chapter 12 for heat exchangers; Chapter 13 for separation towers; Chapter 14 on pumps, compressors, and expanders; and Chapter 15 on chemical reactor design, focusing on modeling situations in which plug flow and perfect back-mixing assumptions do not hold. The last two chapters of Part II deal with equipment sizing and costing (Chapter 16) and profitability analysis (Chapter 17).

Part III discusses the analysis tools required for both product design and process design; the first two chapters cover analysis in product design. Chapter 18 provides a guide to six-sigma design strategies, which offer a means to improve product quality through the identification of the root causes of variance and their subsequent attenuation. Chapter 19 focuses on the relationship between product technical specifications and the design of the manufacturing plant and discusses issues such as product pricing and demand. Part III also consists of three chapters supporting analysis in process design, starting with Chapter 20 on plantwide controllability assessment followed by Chapter 21 on design optimization and Chapter 22 on the design and scheduling of batch processes.

Part IV describes design reporting in Chapter 23, emphasizing product and process design aspects, with a template provided for writing design reports and with recommendations for preparing oral presentations.

The last part of the book, Part V, is a collection of case studies: three featuring products and one featuring a process. Each of the three product design case studies begins with a discussion of new related technologies. Then, the most important product design steps are covered. Each case study involves some engineering design calculations and/or lab data regression to be performed by students. The process design case study involves the design process for the manufacture of ammonia and describes the development of an initial feasible, but rather unprofitable, base-case design, and then shows how the initial design is systematically refined until it is acceptable.

LIMITED TIME—PROCESS OR PRODUCT DESIGN?

When limited time is available, some faculty and students may prefer to focus on *process* design rather than *product* design by following the flow chart in Figure i-1. This can be accomplished by beginning in Part I with the introduction in Chapter 2 and coverage on design literature, innovation, energy sources, environmental sustainability, safety, and ethics in Chapter 3; then, Chapters 6–11 from Part II systematically cover heuristics, process simulation, reactor and separation system design, second-law analysis, and heat and power integration. The sequence in Chapters 12–15, detailing equipment design, may be left to students as self-study in connection with their design project work, or portions may be covered in class. Some universities teach process economics as a separate course, but those that do not will need to include Chapter 16, covering cost accounting and capital cost estimation, and Chapter 17, covering profitability analysis. Finally, all or part of the sequence of three chapters from Part III can be included: Chapter 20 on plantwide controllability assessment (probably the most important of the three to cover), Chapter 21 on design optimization (if not covered elsewhere, for example, in a course on numerical methods), and Chapter 22 on the design and scheduling of batch processes. Part IV, covering design reports, should be left to self-study. The case study in Chapter 27 could be used either by students for self-study or could be the subject for a constructive class discussion with students as preparation for their design project work.

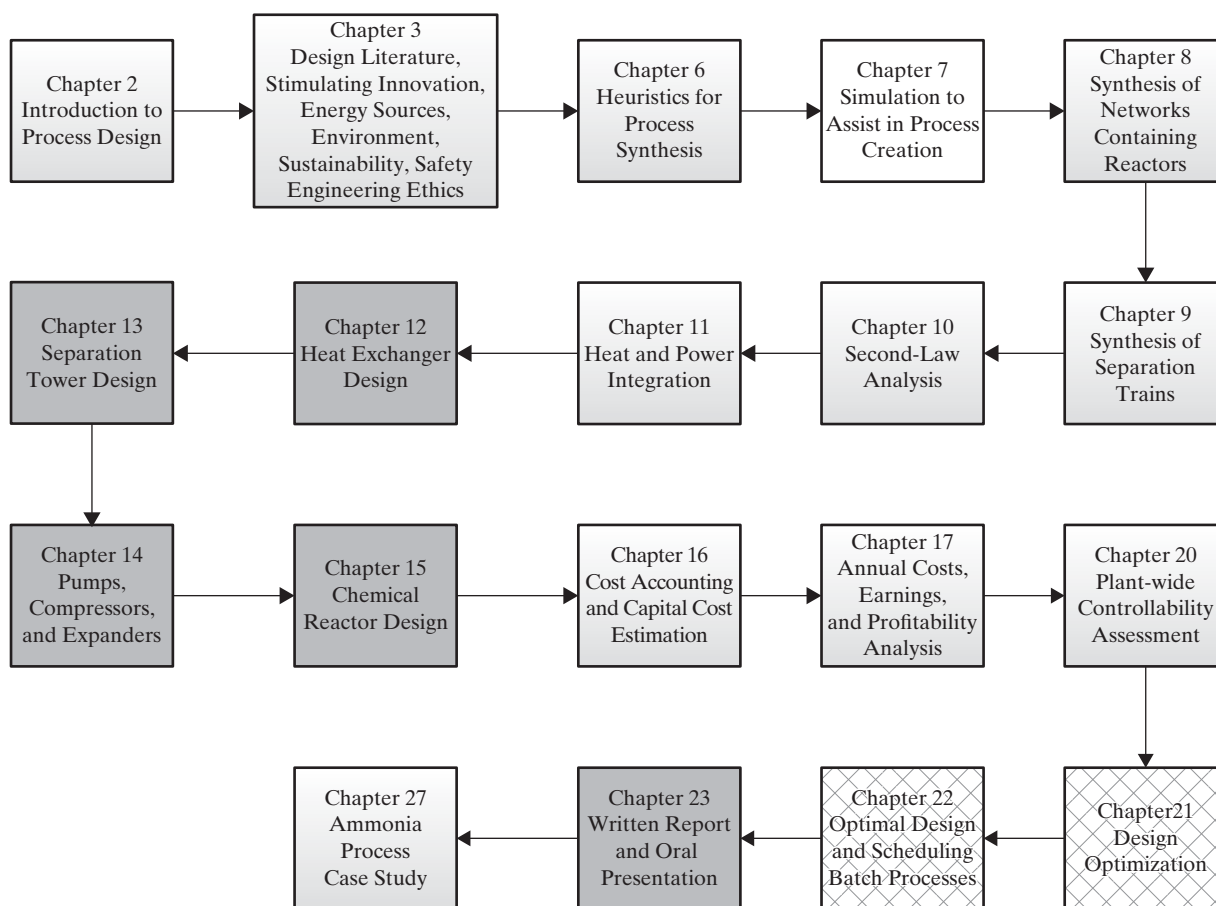


Figure i-1 Process design chapter sequence: Chapters for potential self-study are indicated in grey with optional materials indicated in cross-hatched boxes.

Courses that focus on *product* design rather than *process* design can proceed as shown in the flow chart in Figure i-2, starting with the introduction in Chapter 1 followed by materials on the design literature, innovation, energy sources, the environment, sustainability, safety, and ethics in Chapter 3. These could be followed by the two chapters on product design synthesis in Part II on the design of molecules and mixtures (Chapter 4) and on formulated products and devices (Chapter 5). Chapter 19 on decision making in product development should be covered next and then Chapters 21 on design optimization (assuming it is not covered elsewhere) and Chapter 22 on optimal design and scheduling of batch processes. It would be helpful to end the course with detailed coverage of the case studies in Chapters 24–26. As with the process design sequence, it is recommended that Part IV covering design reports be left to self-study.

FORMAT OF COURSEWARE AND SUPPORTING WEB SITE

This courseware takes the form of a conventional textbook now available for the first time as an e-book. Because the design strategies have been elucidated during the development of this courseware, fewer specifics have been provided in the chapters concerning the software packages involved. Instead, a multimedia encyclopedia has been developed to give many examples of simulator input and output with frame-by-frame instructions to discuss the nature of the models provided for the processing units, and it presents several example calculations. The encyclopedia uses voice, video, and animation to introduce new users of the steady-state simulators to the specifics of two of the most widely used process simulation programs, ASPEN PLUS and UniSim® Design, as well as instruction in MATLAB. These programs include several tutorials that provide instruction on the solution of problems for courses in mass and energy balances, thermodynamics, fluid mechanics, heat transfer, separations, and reactor design. In many cases, students will have already been introduced to the

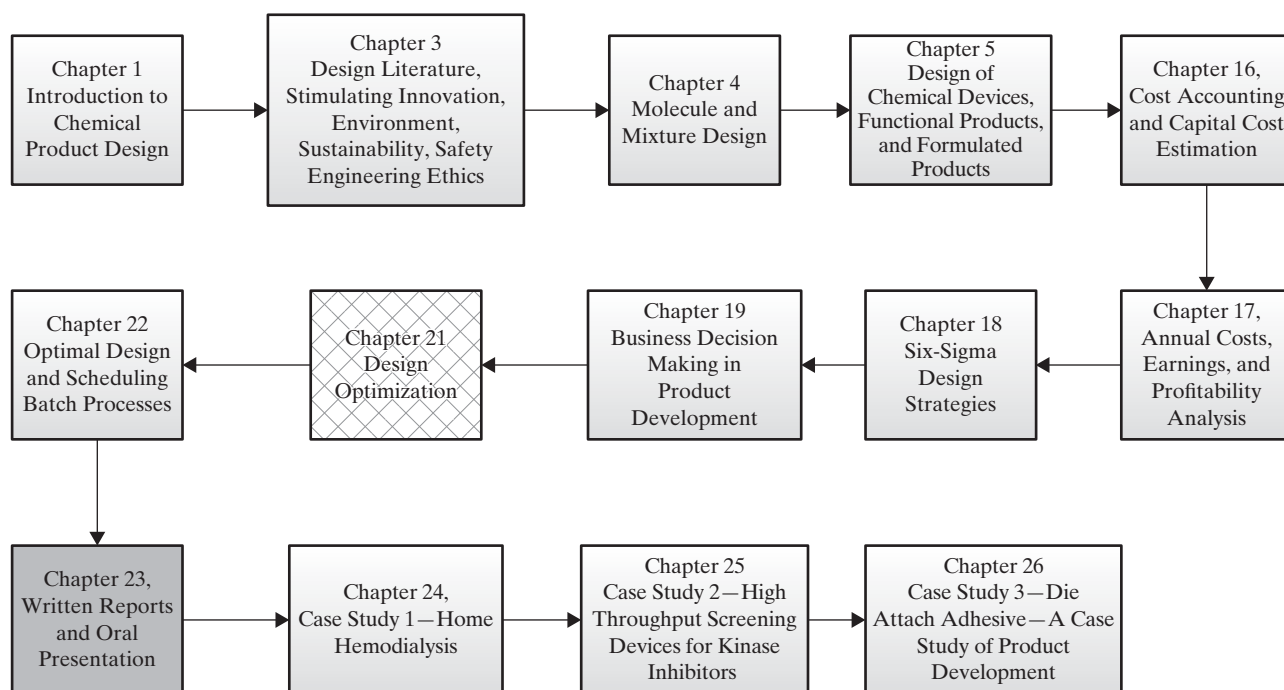


Figure i-2 Product design chapter sequence: Chapters for potential self-study are indicated in grey with optional materials indicated in cross-hatched box.

process simulators in these courses. Also, video segments show portions of a petrochemical complex in operation, including distillation towers, heat exchangers, pumps and compressors, and chemical reactors. The Wiley site¹ that supports this book also includes files that contain the solutions for many examples using either ASPEN PLUS or UniSim® Design as well as the MATLAB scripts in Chapter 20. The files are referred to in each example and can easily be used to vary parameters and to explore alternative solutions.

Supplemental sections of several chapters are provided in PDF files on the Wiley site that supports this book with only a brief summary of the material presented in the textbook. Furthermore, Appendix II lists design projects whose problem statements are provided in a PDF file on a University of Pennsylvania site.² These involve the design of chemical processes in several industries. Many are derived from the petrochemical industry with much emphasis on environmental and safety considerations, including the reduction of sources of pollutants and hazardous wastes and the purification before streams are released into the environment. Several projects originate in the biochemicals industry, including fermentations to produce pharmaceuticals, foods, and chemicals. Others involve the manufacture of polymers and electronic materials. Each design problem has been solved by groups of two, three, or four students at the University of Pennsylvania; copies of their design reports are available by Interlibrary Loan from the University of Pennsylvania Library. Since 2011, PDF files are also available from the University of Pennsylvania Library.

ADVICE TO STUDENTS AND INSTRUCTORS

In the use of this textbook and accompanying matter, students and instructors are advised to take advantage of the following features:

Feature 1: Well-organized Sequence of Materials to Teach Product Design

This textbook introduces the key steps in *product* design with numerous examples. These steps have been developed with the assistance and recommendations of successful practitioners of product design in industry. Students can begin with the overview in

¹he-cda.wiley.com/WileyCDA/HigherEdTitle/productCd-0471216631.html.

²www.seas.upenn.edu/~dlewin/UPenn Design Problem Statements.html.

Chapter 1, which introduces the main steps involved in designing products. Computer-aided tools for design of single molecule products and of liquid mixtures and blends are covered in Chapter 4. In Chapter 5, the design of B2C chemical products for which chemical reaction and transport phenomena tend to play a dominant role is discussed in detail. The discussion of business decision making for B2C products, which is discussed in Chapter 19, is more involved than that for B2B products. Three detailed case studies for chemical products are presented in Chapters 24, 25, and 26. These examples can be expanded and/or used as the basis of design projects for student design teams. In our experience, students can frequently formulate their own product design projects based on their own experience and awareness of consumer needs.

Feature 2: Well-organized Sequence of Materials to Teach Process Design

Process synthesis is introduced primarily using heuristics in Chapters 2 and 6, whereas Chapters 8–11 provide more detailed algorithmic methods for chemical reactor network synthesis, separation train synthesis, and heat and power integration. Chapter 7, covering process simulation, provides the basis for testing process design alternatives.

This feature enables the student to begin process designs using easy-to-understand rules of thumb. Once these ideas have been mastered, students can learn algorithmic approaches that enable them to produce better designs. For example, consider how students would design a plant to produce a commodity chemical, say ammonia, from suitable raw materials—in this case, natural gas and air. Chapter 2 introduces process design focusing on the generation of a feasible base-case design, that is, one that satisfies production demands with respect to quantity and quality without necessarily being profitable. Most, if not all, of the decisions made at this point rely on heuristics, which are introduced in Chapter 2 and covered more thoroughly in Chapter 6. Because the implementation and testing of design ideas are carried out using process simulation, this is supported by the systematic coverage of the efficient use of process simulation in Chapter 7, as well as in the multimedia encyclopedia that is available on the Wiley Web site that supports this book. Attempts to improve profitability use methodologies for reactor network synthesis described in Chapter 8 (one of the examples in that chapter shows how to optimally operate a cold-shot ammonia converter) and separation network synthesis presented in Chapter 9 (although not important for ammonia synthesis). At this stage, students should be ready to learn about how heat integration can improve their design; Chapter 11 provides them a comprehensive guide, which also includes worked examples directly relevant to the problem(s) at hand. Cost accounting and profitability analysis are handled formally in Chapters 16 and 17, which provide a basis for estimating the degree to which their process is cost effective. This whole sequence can be used to support an entire design project as illustrated in Chapter 27, a case study that goes through the entire design process for a plant to produce 450 MTD of ammonia.

Feature 3: Instruction in the Use of Simulators

Throughout this courseware, various methods are used to perform extensive process-design calculations and provide graphical results that are visualized easily including the use of computer programs for simulation and design optimization. The use of these programs is an important attribute of this courseware. We believe that our approach is an improvement over an alternative approach that introduces the strategies of process synthesis *without computer methods*, emphasizing heuristics and back-of-the-envelope calculations. We favor a blend of heuristics and analysis using the computer by augmenting the heuristic approach with an introduction to the analysis of prospective flowsheets using industrial-quality simulators, such as ASPEN PLUS, HYSYS.Plant, UniSim[®] Design, PRO-II, CHEMCAD, FLOWTRAN, BATCH PLUS, and SUPERPRO DESIGNER. These simulators permit access to large physical property, equipment, and cost databases and the examination of aspects of numerous chemical processes. Simulators facilitate the search for optimal operating conditions to improve profitability. Emphasis is on the use of simulators to obtain data and perform tedious engineering calculations. Today, most schools use one of these simulators but often without adequate teaching materials. Consequently, the challenge for us in the preparation of this courseware was to find the proper blend of modern computational approaches with simple heuristics.

Through the use of the process simulators, which are widely used in industry, students learn how easy it is to obtain data and perform routine calculations. They learn effective approaches to building knowledge about a process through simulation. The courseware provides students the details of the methods used for property estimation and equipment modeling. They learn to use simulators intelligently and to check their results. For example, in Chapter 2, examples show how to use simulators to assemble a preliminary database and to perform routine calculations when computing heat loads, heats of reaction, and vapor–liquid equilibria. In Chapter 7, two examples show how to use the simulators to assist in the synthesis of toluene hydrodealkylation and monochlorobenzene separation processes. Most of the remaining chapters show examples of the use of simulators to obtain additional information, including equipment sizes, costs, profitability analyses, and the performance of control systems.

Because the book and the accompanying materials contain many routine self-study examples of how the simulators are useful in building a process design, the instructor has time to emphasize other aspects of process design. Through the examples and multimedia encyclopedia with emphasis on ASPEN PLUS and UniSim[®] Design, students obtain the details they need to use the simulators effectively, saving the instructor time in class and in answering detailed questions as students prepare their designs. Consequently, students obtain a better understanding of the design process and are exposed to a broader array of concepts in process design. In a typical situation when creating a base-case design, students use the examples in the text and the encyclopedic modules and the tutorials to learn how to obtain physical property estimates, heats of reaction, flame temperatures, and phase distributions. Then, students learn to create a reactor section using the simulators to perform routine material and energy balances. Next, students create a separation section and may eventually add recycle streams. Thanks to the coverage of the process simulators in Chapters 2 and 7 and the supporting materials, the instructor needs to review only the highlights in class.

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Introduction to Product and Process Design

Engineers apply science and mathematics to provide technological solutions to human and societal needs. The solutions are most often in the form of devices, machines, materials, processes, structures, and systems. The solutions are achieved by research, development, design, and operation. Chemical engineers are unique in their ability to solve technical problems using the principles of chemical kinetics, chemical and physical thermodynamic equilibrium, and mass transfer in addition to the principles of heat transfer and fluid mechanics also applied by other engineers. This textbook applies these principles to chemical **product design** and chemical **process design**.

Product design, introduced in Chapter 1, refers to product design and development steps for both business-to-business (B2B) products and business-to-consumer (B2C) products. Examples of B2B chemical products are (1) polyethylene terephthalate (PET) bottles, (2) nylon fiber, (3) PyrexTM boro-silicate glass, and (4) polyvinyl butyral. Examples of B2C chemical products are (1) sunscreen lotions, (2) insect repellent sprays, (3) light-emitting diode (LED) bulbs, (4) hemodialysis devices for home use, and (5) high throughput screening devices for kinase inhibitors.

Product design consists of a product formulation or construction and a prototype of the product suitable for testing and evaluation. The product construction shows the arrangement of product elements with specified dimensions and desired physical and chemical properties. Chemical engineers work closely with chemists, physicists, and/or material scientists to develop product formulations or construction and are responsible for combining the materials and processing technology to deliver desired product characteristics and performance.

Product development includes other nontechnical aspects of gathering customer needs, opportunity assessment, buy-or-make decision, product cost target and pricing, and sale and marketing strategy needed to launch

a new product. Chemical engineers work closely with the business, legal, manufacturing, and supply-chain professionals to design a product that meets the desired cost target.

Process design, introduced in Chapter 2, refers to multiple-step chemical processes for converting raw materials into desired chemicals. The steps may include chemical reactors; equipment to separate chemical mixtures and phases; heat exchangers to set temperatures and phase conditions; and pumps, compressors, and turbines to set pressures. The process may operate continuously, batchwise, or semicontinuously. Examples of processes include the manufacture of (1) gasoline, diesel fuel, lubricants, fuel oils, and so on from crude oil; (2) vinyl chloride from ethylene and chlorine; (3) the potassium salt of penicillin V from phenoxyacetic acid, aqueous glucose, and cottonseed oil; and (4) ammonia from ambient air and natural gas.

A process design is presented in a process-design report that (PFD) showing the arrangement of the selected equipment with their connecting streams; the temperature, pressure, chemical composition, and total flow rate or amount of the material into and out of each piece of equipment; and the rate or amount of energy into or out of each piece of equipment. The PFD is accompanied by tables of stream component flow rates, stream properties, energy requirements, and equipment specifications including recommended materials of construction as well as a complete description of the process and a diagram showing process instrumentation and controllers.

Except perhaps for small projects, **plant design** is largely the province of civil, electrical, and mechanical engineers who take the information in the process-design report and do all other engineering design necessary to construct the plant, including the determination of plant location; design of the plant layout; selection and design of storage vessels for raw materials and products; detailed design of processing equipment; design of supporting structures and foundations for the equipment, design of piping and ducting

systems; selection of utilities (cooling water, compressed air, electricity, fuel oil, steam, etc.), and other service facilities. During plant design, chemical engineers may be involved in the detailed design of equipment involving chemical considerations, preparation of a piping and instrumentation diagram (P&ID), and plant layout decisions (at least where safety is a concern). Except for the most common types of processing equipment (heat exchangers, separation columns, pumps, compressors, expanders, and

reactors), engineering design aspects of plant design are not treated in this textbook.

Chapter 3 of Part I discusses some supporting aspects of product and process design, including use of the design literature, stimulation of innovation, energy sources, environmental and safety considerations, sustainability with nature, and engineering ethics. The details of product and process design are presented in subsequent parts of this textbook.

Chapter 1

Introduction to Chemical Product Design

1.0 OBJECTIVES

This chapter introduces an overview of the myriad chemical products a chemical engineer designs and develops. Launching a chemical product into the market is a complex process. The tasks that need to be executed in a typical product-development project, partly in collaboration with professionals in other disciplines, are identified. The methodologies and tools for performing such tasks are discussed and illustrated with several examples.

After studying this chapter, the reader should:

1. Be cognizant of the diversity of chemical products.
2. Know the different classes of chemical products and be familiar with some representative products and their characteristics.
3. Appreciate the overall approach to product design from conceptualization to product launch.
4. Be aware of the contributions a chemical engineer can make in product design and development.
5. Be familiar with some of the tools and methodologies used in product design and development.

1.1 INTRODUCTION

The chemical industry is a vast industry with a wide variety of more than 70,000 products, including agrichemicals, ceramics, elastomers, electronic materials, explosives, foods, flavors and fragrances, fuels, industrial gases, inorganic chemicals, metals, oleochemicals, petrochemicals, pharmaceuticals, plastics, and textiles. The industry powers economic growth and raises the standard of living of modern society (Arora et al., 1998). A typical chemical engineering undergraduate curriculum initially focuses on the basics of “how to make” and primarily on organic chemicals. Thus, chemical reactors and unit operations such as distillation, crystallization, absorption, and extraction are covered in detail. Chemical kinetics, transport phenomena—heat, mass, and momentum transfer, and thermodynamics—provide the fundamental understanding of the way in which these operations function.

We consider in Chapter 1 “what to make,” which is perhaps the most important decision for the management of a firm. To make a profit, all firms, public or private, large or small, have to produce products that the customer is willing to buy. With the rapid changes in technology, societal needs, consumer expectations, and competitive forces, new products have to be invented and existing products have to be improved or reduced in cost for a firm to prosper or merely to stay in business.

1.2 THE DIVERSITY OF CHEMICAL PRODUCTS

Chemical products are ubiquitous in our daily lives. We may begin the day using a soap bar and shampoo to wash up, brushing our teeth with a toothbrush and tooth paste, and moisturizing our face and hands with a lotion. The clothes we put on may be

made of synthetic fibers. In our home, we may find processed foods such as ice cream and butter in the refrigerator, shortening and cooking oil in kitchen cabinets, pharmaceuticals in the medicine cabinet, nylon or polyester carpet on the floor, paint on the walls, a polymer composite countertop, and lawn fertilizer in the storage shed. In some households, there may be an air purifier with titanium dioxide, which is capable of catalytically decomposing the volatile organic compounds in the air and an air conditioner with an environmental friendly refrigerant. Going to work by automobile, we find gasoline in the gas tank, tires made of styrene-butadiene rubber, and a shatterproof glass windshield with an interlayer of transparent polyvinyl butyral.

The Chain of Chemical Products

All the products mentioned above are derived from nature—air, natural gas, petroleum (also known as crude oil), minerals, plants, and animals. Figure 1.1 is a highly simplified chemical product chain showing how the chemical products are produced successively from natural resources. For example, nitrogen can be obtained by cryogenic distillation of air whereas hydrogen is obtained from natural gas. Reaction between nitrogen and hydrogen by the Haber-Bosch process produces ammonia (see Chapter 27). Ammonia in turn reacts with carbon dioxide, also obtained from natural gas, to form urea, which is a key component in fertilizer.

A wide range of hydrocarbons such as ethylene, butadiene, benzene, toluene, xylene, and alkenes are obtained from petroleum in a refinery. In the petrochemical industry, these hydrocarbons can be used to produce a myriad of other useful chemicals. For example, ethylene, the largest chemical product

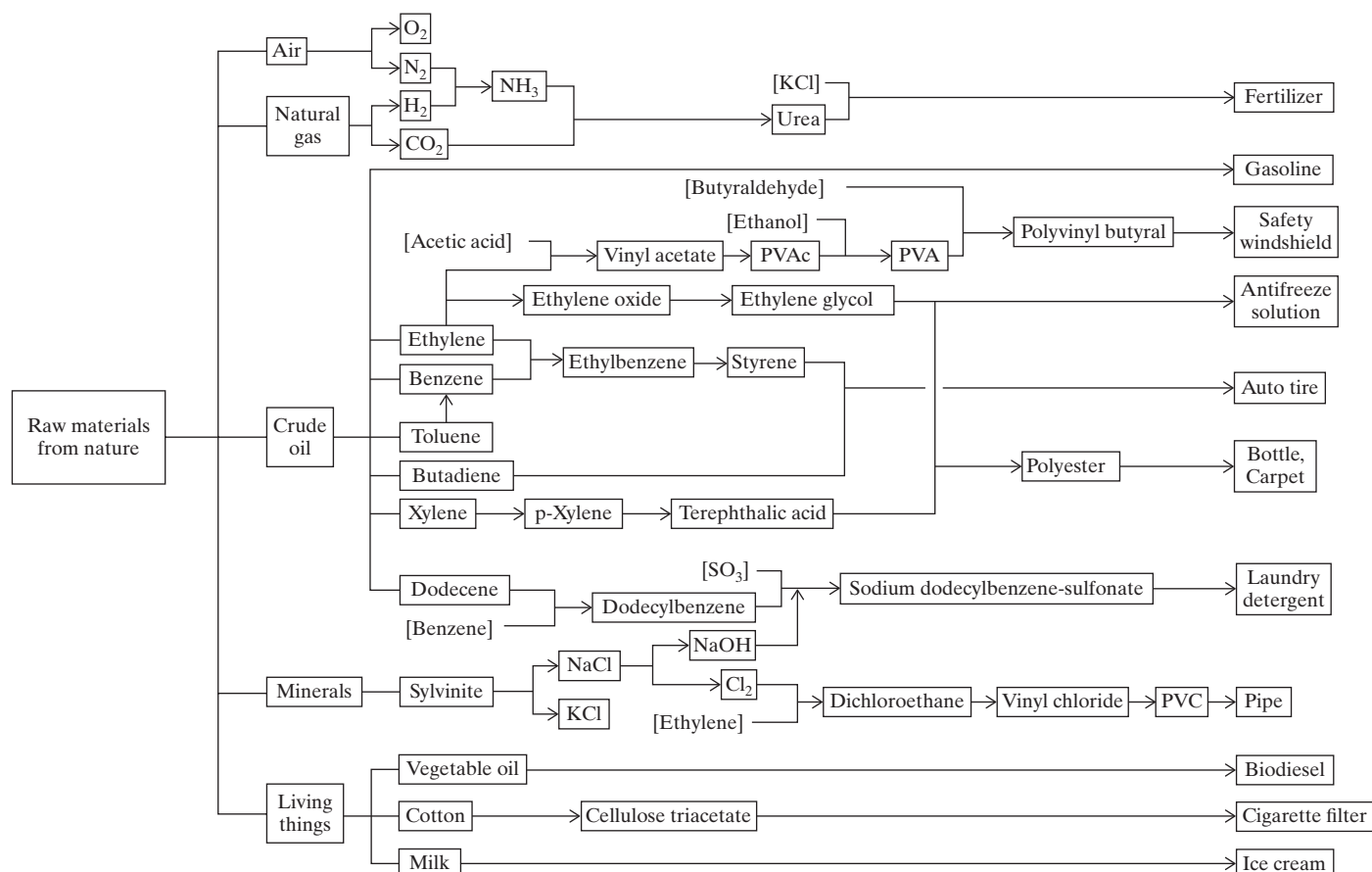


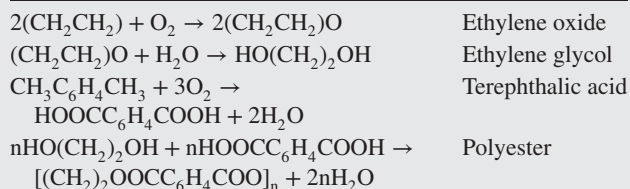
Figure 1.1 A small subset of the chain of chemical products. (The chemicals in the brackets are those not included or out of order in the product chain.)

by volume, is used in the production of rubber, plastics, solvents, and so on. It reacts with acetic acid to form vinyl acetate. Polyvinyl acetate (PVAc) reacts with ethanol to form polyvinyl alcohol (PVA). Polyvinyl butyral, the interlayer of shatterproof glass windshields, is made by reacting PVA with butyraldehyde. Ethylene can also be oxidized to ethylene oxide, which is hydrolyzed to ethylene glycol. Ethylene glycol is used in an antifreeze solution. Ethylene can also react with benzene to form ethylbenzene. Dehydrogenation of ethylbenzene forms styrene. Many automobile tires are made from various types of styrene-butadiene rubber. Sometimes, the inherent amount of benzene in the crude oil is insufficient to meet what is required in the downstream products whereas toluene is in excess. In this case, the excess toluene is converted to benzene using a process called hydrodealkylation, which is discussed in Chapter 6. Xylene contains three isomers: para-, ortho-, and meta-xylenes. Because only para-xylene is oxidized to terephthalic acid, para-xylene has to be separated from the mixture of isomers. After first removing ortho-xylene by distillation, para-xylene can be purified from para- and meta-xylene by crystallization or adsorption. A condensation reaction between terephthalic acid and ethylene glycol forms polyethylene terephthalate (PET), which is used in products such as floor carpet. PET is also used to make transparent bottles by injection molding. Dodecene, one of the alkenes in crude oil, can be converted to sodium dodecylbenzenesulfonate by reacting with benzene, sulfur trioxide, and sodium hydroxide, successively. Sodium dodecylbenzenesulfonate is a member of

the linear alkylbenzenesulfonates, a major component of laundry detergent.

EXAMPLE 1.1 Show the main chemical reactions for producing polyester starting with ethylene and para-xylene

SOLUTION



As another example, a mineral such as Sylvinitite, a mixture of sodium chloride and potassium chloride, can be separated into its constituent components. Sodium chloride undergoes the chlor-alkali process to produce sodium hydroxide and chlorine. Ethylene reacts with chlorine to form dichloroethane, which is pyrolyzed to vinyl chloride, as discussed in Chapter 2. Polymerization of vinyl chloride forms polyvinylchloride (PVC), which is widely used for making pipes. Potassium chloride is used as a fertilizer.

Surfactants for soaps and detergents can also be obtained from plant oils and animal fats, which are esters of glycerol and fatty acids. Biodiesel, consisting of long-chain alkyl esters, can also be produced from plant oils. Cotton fibers are often blended with polyester fibers in a fabric for clothing. The blended fabric offers the natural feel of cotton while adding the strength and durability of polyester. Cellulose triacetate from cotton linters is used as a semipermeable membrane for water purification. A wide variety of dairy products such as cheese, ice cream, and yogurt are produced from animal milk.

Many excellent books have been written on industrial chemicals similar to those described here; see, for example, Faith et al. (1975), Austin (1984), and Chenier (2002). Books are also available on those chemical products at the end of the product chain that are used by the consumers (Cussler and Moggridge, 2011; Bröckel et al., 2007, 2013; Ng et al., 2007; Wesselingh et al., 2007).

Companies Engaging in Production of Chemical Products

The chain, or more appropriately, the network in Figure 1.1 captures only a very tiny segment of an exceedingly complex network made up of tens of thousands of products. Typically, a company focuses on a certain segment of this product chain. The separation and use of gases is dealt with by *gas companies* such as Linde, Air Products, Praxair, and Air Liquide. Petroleum exploration and refining the recovered oil into different chemicals are handled by the so-called *oil companies* such as Saudi Aramco, Exxon-Mobil, British Petroleum, and Petro China. BASF, Sinopec, Dow, SABIC, DuPont, and Mitsubishi are referred to as *chemical companies*; they convert raw materials and chemicals from oil companies into more complex compounds. Drug discovery is so challenging that it is often handled by highly specialized *pharmaceutical companies* such as Pfizer and Merck. Mineral processing tends to be handled by focused companies as well. For example, Potash Corp is the world's largest producer of potassium chloride (also known as potash). Products such as soaps, detergents, and lotions as well as some processed foods are manufactured by *consumer goods companies* such as Procter & Gamble and Unilever. In general, the companies upstream of the chemical product chain are relatively large to take advantage of economies of scale. The companies closer to actual consumers are smaller because these downstream companies have to react swiftly to meet market demands. Indeed, many small to medium-size companies produce a broad array of products such as humidity sensors, medical diagnostic kits, and fabric softeners, among others.

B2B and B2C Chemical Products

The products in the chain of chemical products can be broadly classified into two classes: *business-to-business (B2B)* and *business-to-consumer (B2C)*. The former involves a transaction between two businesses, and the latter involves a sale to the consumer. Most of the oil companies' products are B2B products. For example, chemicals such as para-xylene and butadiene are supplied to the chemical companies as raw materials. These chemical products are often referred to as *commodity chemicals*

because the chemical company buys such chemicals from any supplier at the lowest price possible provided that these products meet the company's raw-material specifications. Often, the primary concern for commodity chemicals is purity. The empty PET bottle that the polymer processing company sells to the bottling company is an *industrial product*; it is still a B2B chemical product but is no longer a chemical. When a consumer purchases a bottle of distilled water, the quality of terephthalic acid, a compound in the product chain leading to the PET bottle, is not the consumer's concern. However, the oxidation of para-xylene to terephthalic acid, if not done properly, produces a colored compound, 4-carboxybenzaldehyde, which makes the PET bottle yellowish. Thus, although commodity chemicals might seem remote from the consumer, their product specifications are indirectly influenced by the consumer, who is the ultimate user of the chain of products. The term *basic chemicals* is used synonymously as commodity chemicals because they are the building blocks of more complex molecules. Many novel molecules with special characteristics are derived from the basic chemicals and are produced in relatively small quantity. They belong to the class of *specialty chemicals*, which are sold based on what they can do and often offer a relatively higher profit.

The consumer has a more direct say on the specifications of B2C products, or alternatively, *consumer products*, such as shampoo, lotions, processed foods (butter, cheese, yogurt, potato chips), halogen light bulbs, masking tapes, face masks, and air purifiers. Some of the specifications are quantitative. For example, the air purifier has to be able to reduce the concentrations of certain impurities in the air of a closed room of a certain size to below specified values within a given period of time. Often, the specifications are qualitative in nature. The product has to offer consumer delight—feelings of the consumers when their expectations are fully satisfied. For example, a lotion has to feel smooth and smell good, a wine has to possess a desired bouquet, and a detergent has to impart a soft feel to the fabric. The product specifications for consumer products are often referred to as *product attributes* to reflect some of the qualitative desires. Example 1.2 shows the typical product attributes for creams and pastes (Wibowo and Ng, 2001). In addition, the product has to be safe and environmentally friendly. These seemingly obvious prerequisites can become controversial. For example, there has been a heated debate on the safety and disposal of PVC. There is no absolute safety, and it is difficult to get all parties to agree on how safe is sufficiently safe.

EXAMPLE 1.2 Typical product attributes for creams and pastes

Creams and pastes such as moisturizing cream and sunscreen lotion are common consumer products. Provide a list of their typical product attributes.

SOLUTION

There are four typical product attributes:

Functional

Protects parts of the body

Cleans parts of the body

Provides a protective or decorative coating
 Causes adhesion to body surface
 Delivers an active ingredient to the target area

Rheological

Can be poured easily
 Spreads easily when rubbed on skin
 Does not flow readily under gravity but is easy to stir
 Should give a uniform coating when applied to surface
 Should not flow by itself but can be squeezed out of the container

Physical

Must be stable for a period of time
 Melts at a certain temperature
 Must release an ingredient at a controlled rate

Sensorial

Feels smooth
 Does not feel oily
 Appears transparent, opaque, or pearlescent
 Does not cause irritation

Table 1.1 compares different aspects of B2B and B2C chemical products. B2B chemical products change hands in business-to-business transactions. Thus, an oil company sells para-xylene to a chemical company to make PET. The chemical company in turn sells the PET to a polymer processing company to make PET bottles. Most of these B2B products are in relatively pure form because they are the feedstocks for more complex molecules. An obvious exception is gasoline, which is a mixture of hydrocarbons that is sold directly to the consumer at gas stations. In contrast, most B2C chemical products such as detergent and lotion are mixtures that use chemicals from chemical companies such as surfactants and fragrances as ingredients. Some of these mixtures are randomly mixed, but some possess a specified structure. For example, CdS/ZnS quantum

dots have a spherical core of CdS encapsulated by a ZnS shell. B2B product design is primarily a molecular design with considerable input from chemists whereas B2C product design often involves multicomponent systems with or without a structure. The technology involved in B2B products tends to be primarily chemistry and chemical engineering in nature. In a typical herbicide development team of 10 or so researchers, there are often nine chemists responsible for organic synthesis and only one chemical engineer in charge of product and process design. B2C products such as air purifiers or health drinks are likely to involve a more diverse team of technical personnel, including electrical and mechanical engineers and food scientists. Furthermore, for most new products, companies' marketing, financial, and legal teams are often involved to ensure that the relevant issues are properly managed.

In general, the B2B product lifetime is much longer than the B2C product lifetime. This is because the specifications for B2B products tend to be well established and remain unchanged over a long period of time whereas the B2C product attributes evolve rapidly along with the changes in consumer preferences. Figure 1.2 contrasts the product life cycle of a typical B2B product with that of a typical B2C product. It shows that the revenue of a B2B product declines because other competitors enter

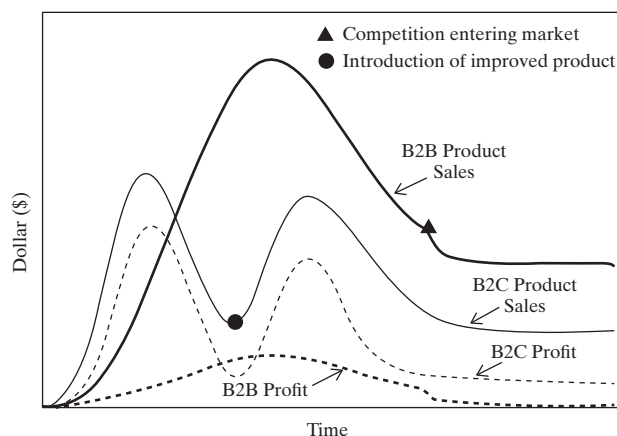


Figure 1.2 Typical life cycles of business-to-business and business-to-consumer chemical products.

Table 1.1 Comparison of Business-to-Business and Business-to-Consumer Chemical Products

	B2B Products	B2C Products
Customers	Allied chemical industries	Consumers
Nature of products	Simple or complex molecules	Devices (equipment), functional products, and formulated products
Product design	Molecular design	Selection of ingredients, product structure, and product attributes
Product life cycle	Decades	Month/year
Team	Primarily chemists and chemical engineers	A multidisciplinary team of marketing personnel, financial specialists, lawyers, electronic engineers, mechanical engineers, chemists, and chemical engineers
Financial goal	Cost reduction	New sources of revenue
Unit operations	Traditional: distillation, crystallization, extraction, absorption, adsorption, etc.	Unconventional: granulation, milling, nanomization, etching, lamination, physical vapor deposition, inkjet printing, screen printing, laser scribing, etc.
Knowledge/know-how	Well structured	Fragmented so far
Technical focus	Engineering optimization	Improved performance followed by reduced cost

the market. The B2C product lifetime is much shorter. The profit relative to sales tends to be much higher than that of the B2B products. In addition, as shown by the two peaks, this B2C product gets a second wind by introducing an improved version.

Because of the long lifetime of commodity chemicals, the research and development (R&D) for B2B products focuses on lowering the production cost of these products whereas the R&D for B2C products emphasizes the conceptualization of new and improved products to generate fresh revenue streams. Most of the manufacturing processes for B2B products are traditional processes. Reaction engineering and unit operations for the manufacturing processes of commodity chemicals including distillation, crystallization, extraction, absorption, adsorption, filtration, membrane separation, and others are well covered in a typical chemical engineering curriculum. The knowledge of commodity chemicals is well structured. The thermodynamic properties of most commodity chemicals are available in the thermodynamic database of commercial simulators. Techniques for predicting the properties of new B2B chemicals are available. If a consumer product is a mixture without a structure such as a liquid fabric softener, processing can be simply mixing operations. For consumer products with a structure, such as solar cells and lithium ion batteries, unconventional processing techniques such as granulation, sputtering, inkjet printing, screen printing, etching, calendaring, and so on can be involved. The technical focus of B2B products, except for new molecules, tends to be process optimization; the technical focus of B2C products tends to be the use of advanced materials or technologies to make products with new or improved attributes for the consumer.

Market Sectors and Classes of Chemical Products

Chemical products can be classified by market sector in which a number of firms sell similar goods and services, and by three product classes which include (1) simple or complex molecules, (2) devices (or equipment) and functional products that perform a desired purpose or function, and (3) formulated products that are obtained by mixing selected ingredients that as a whole offer the desired product attributes. Table 1.2 shows examples of chemical products in each of the three product classes in nine market sectors. Remarks are made (in parentheses) to products that might be unfamiliar to the reader. The examples for devices (equipment) are italicized to distinguish them from those for functional products. Consider agricultural products. They can be new molecules that function as herbicides or pesticides. Microencapsulation of herbicide with ethylcellulose produces a controlled-release granule, a functional product, that provides prolonged action in the field. A mosquito mat is a small cardboard mat impregnated with an insecticide solution. It releases an insecticide on heating. It also contains a dye that gradually changes color during use to indicate the amount of insecticide that remains in the mat. The company also sells an accessory device, a heater that fits the mat with the rate of heating set in such a way that the evaporation of the mosquito repellent continues over the desired use period. An herbicide mixture should be properly formulated to manage the vegetation in a given locality. Obviously, chemical products

represent only a small fraction of the total agricultural industry, which also includes the sale of wheat, corn, and so on. The rest of Table 1.2 covering other market sectors is left to the reader to explore. It should be emphasized that much thought goes into consumer products. The disposable baby or adult diaper has multiple layers of materials to move the urine away from the skin, yet it is made sufficiently inexpensive to be disposable.

1.3 PRODUCT DESIGN AND DEVELOPMENT

Design is a synthesis activity, meaning that different parts are combined to create a coherent whole that offers functions and characteristics that cannot be found in the individual parts. Because many B2B products are primarily molecules, *product design* is equivalent to the synthesis of new molecules. In the past, a chemist often synthesized molecules with the desired characteristics experimentally by trial and error based on intuition and experience. Nylon, discovered in 1934 by Wallace Carothers at DuPont, is a classic example (Hounshell and Smith, 1988). With recent advances in molecular design (Wei, 2007), computer tools are now available to facilitate the design of molecules as discussed in Chapter 4. Because B2C products are primarily mixtures and devices, *product design* is the activity that aggregates the constituent parts that already exist to generate the final product. Similar to the molecular design tools, computer tools have been developed to predict the properties of mixtures. Computer tools are also available to facilitate the design of the three-dimensional product structures of devices and equipment items such as heat exchangers and distillation columns.

After product design, many activities such as product prototyping and product testing are needed. These activities are referred to as *product development*. Product design and development is inseparable from process design and development to manufacture a product successfully. In addition, marketing, business, and financial specialists as well as engineers from different disciplines are needed to address all relevant aspects. An overview of the activities in a typical product design and development project is presented next.

Tasks and Phases in Product Design and Development

These activities span three phases in time—*product conceptualization (Phase I)*, *detail design and prototyping (Phase II)*, and *product manufacturing and launch (Phase III)*—and can be classified by *job function* in terms of *management, business and marketing, research and design, manufacturing, and finance and economics*. The activities can also be grouped into various *tasks* (such as project management, market study, product design, prototyping), which may last over more than one development phase (Cheng et al., 2009). For example, economic analysis is performed in all three phases and is part of manufacturing as well as finance and economics. Of particular interest are those activities, italicized in Figure 1.3, that require the input of a chemical engineer. The rest of the issues, which are not-italicized, such as product launch are normally handled by personnel from other disciplines and are not discussed further here.

Table 1.2 Different Classes of Chemical Products in Various Market Sectors

Market Sector	Molecules	Devices (Equipment)/Functional Products	Formulated Products
Agriculture	Herbicide Pesticide	<i>Liquid mosquito repellent dispenser</i> Controlled-release herbicide Mosquito repellent mat Plant seeds	Fertilizer mixture Herbicide mixture Insect repellent
Automotive	Polyvinyl butyral Butadiene-Styrene copolymer	Auto tire Safety windshield Sun control window film Diesel exhaust fluid (an aqueous urea solution used with a catalytic system in a diesel vehicle to reduce nitrogen oxides in its exhaust)	Antifreeze Motor oil
Building & Construction	Refrigerant Binder Sealant	<i>Indoor catalytic air cleaner</i> <i>Humidity sensor</i> Smart window (applying voltage to change its light transmission properties) Weather barrier film Acrylic composite countertop Foamed concrete	Paint Adhesives for paneling Stucco
Electronics	Organic light-emitting diode materials Phosphor Fullerenes (as electron acceptor) Graphene	<i>Optical bonding equipment</i> LED light <i>Touch panel</i> Silver nanowire Quantum dot	Optically clear adhesive Die attach adhesive Encapsulant Copper nanoparticle paste
Energy	Lithium iron phosphate, nickel cobalt manganese (battery cathode materials) Biodiesel Bioethanol	<i>Solar panel</i> <i>Fuel cell</i> <i>Battery</i> Battery electrolyte	Heat transfer fluid Drilling mud
Environmental	Coagulant Antiscalant	Ion exchange resin <i>Reverse osmosis membrane</i> <i>Dehumidifier</i>	Air freshener Adsorbents for water filter
Food & Beverage	D-Xylose (commonly called wood sugar. It is a natural 5-carbon sugar obtained from plants. It adds flavors to prepared foods and can be used as animal feed.) Sugar ester (a food grade surfactant with sucrose as hydrophilic group and fatty acid as lipophilic group)	<i>Espresso coffee machine</i> <i>Ice cream machine</i> <i>Wine aerator</i> Textured vegetable protein (meat substitute)	Ice cream Health drinks
Personal Care, Health Care & Medical	Tetrafluoroethane (a propellant for inhalant drug) Active pharmaceutical ingredient	<i>Medical diagnostic kit</i> Nylon toothbrush filaments Herbal extract Transdermal patch Tooth brush Disposable diaper Hand warmer <i>Hemodialysis device</i>	Tooth paste Sunscreen lotion Bar soap Hair spray Fabric softener Laundry detergent powder Pharmaceutical tablet
Packaging & Printing	Ethylene vinyl acetate copolymer (used as a peelable sealing layer)	<i>Flexo platemaking equipment</i> Food packaging film	Ink for digital textile printing Toner for photocopying Screen print paste

Project Management

The starting point of a product-development project is to formulate an *Objective-Time Chart* (Figure 1.4). This is part of the project management task in Phase I. It shows the objectives and subobjectives that have to be met within a given time

horizon. Here, objectives A–E are the high-level objectives. For example, these might include the high-level tasks such as market study, product design, and feasibility study shown in Figure 1.3. In Figure 1.4, objective D is decomposed into objectives D1–D6. For example, if objective D is product design, D1 might be

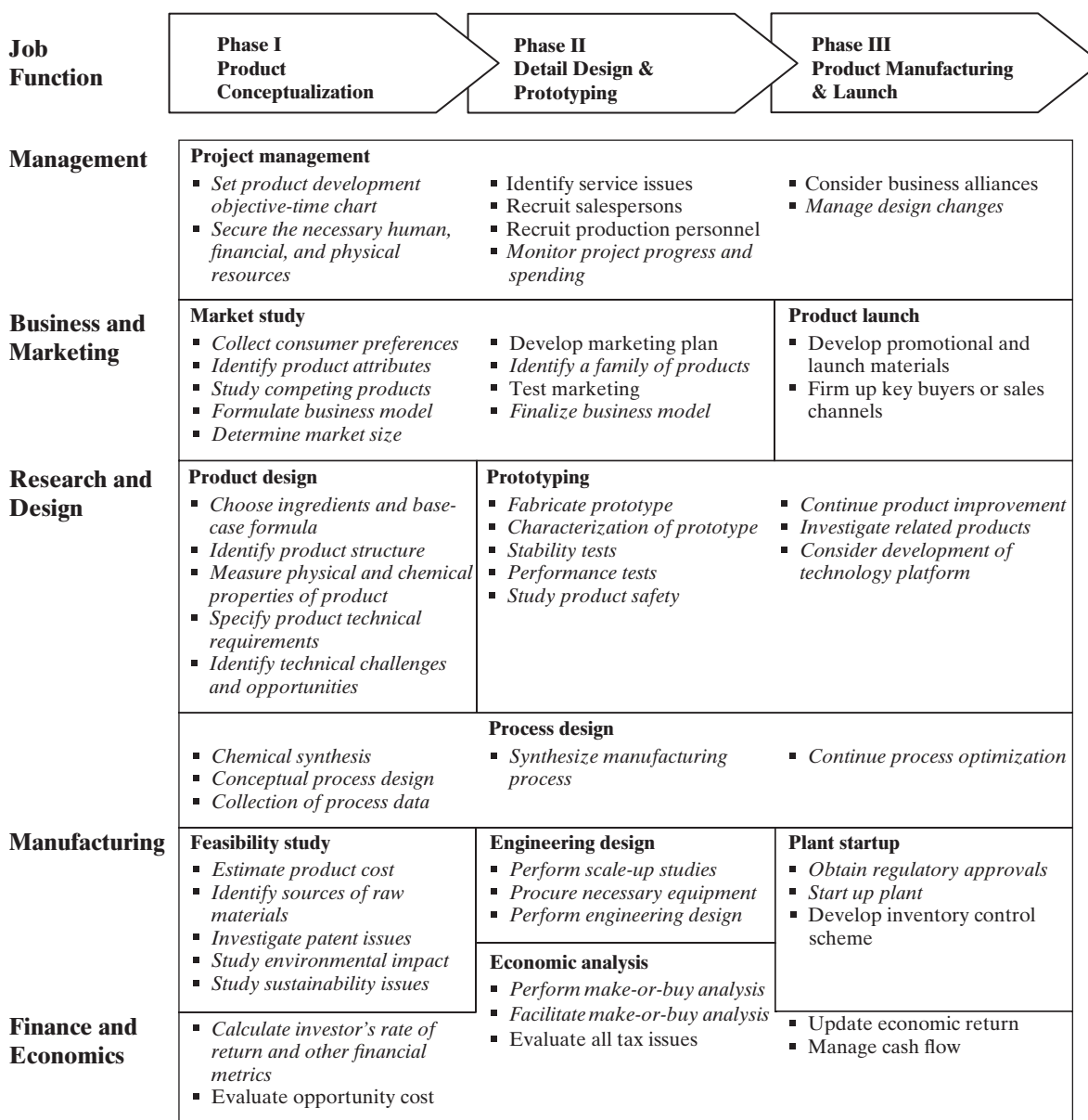


Figure 1.3 The phases and job functions in a multidisciplinary, hierarchical framework for product design and development.

selection of ingredients and D6 measurement of product's physical and chemical properties. Objective D6 is further decomposed into D61–D65. D61 could be measurement of viscosity, D62 measurement of pH, and so on. This methodology is often used by a product/process development team to show all team members the tasks that need to be performed and the time by which they should be completed. By offering a hierarchical view of the development project in its totality, that is, by viewing the whole project with successive layers of increasing details, every member knows what other members are doing to achieve the overall goal. Also, the objective-time chart highlights the tasks that can be carried out concurrently, thereby reducing the overall development time. For example, objectives D2 and D4 take place more or less concurrently and so do D3 and D5.

Different resources are needed to achieve an objective or subobjective. Figure 1.5 depicts *RAT²IO*, a mnemonic acronym

that stands for resources, activities, time and tools, input/output information, and objective. Thus, we identify in advance the *resources* (people and money) required to complete certain *activities* (experiments, modeling, and synthesis) within a specified period of *time* using proper *tools* (experimental setup or software) to generate the necessary *information* and to meet the given *objective*. The deceptively simple objective-time chart in Figure 1.4 is what distinguishes an expert from a novice. An effective project manager with the right experience can draw up a realistic timeline, ensure the availability of the necessary manpower and financial resources, and follow through to facilitate the flow of input/output information from objectives to objectives or to subobjectives. Thus, the manager should have a good appreciation of the *RAT²IO* needed for the various tasks in a product-development project although no individual is expected to master all the details.