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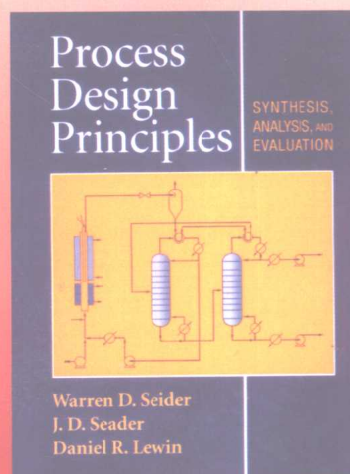
PROCESS DESIGN PRINCIPLES

Synthesis, Analysis, and Evaluation

过程设计原理

——合成、分析和评估

Warren D. Seider J. D. Seader
Daniel R. Lewin



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前 言

随着中国社会主义现代化建设进入新的阶段,以高质量的高等教育培养千百万专门人才,迎接新世纪的挑战,是实现“科教兴国”战略的基础工程,也是完成“十五”计划各项奋斗目标的重要保证。为切实加强高等学校本科教学并提高教学质量,教育部于2001年专门下发文件提出12条意见,对高等学校教学工作从认识、管理、教师队伍到教学方法和教学手段等给予指导。文件强调,按照“教育要面向现代化、面向世界、面向未来”的要求,为适应经济全球化和科技国际化的挑战,本科教育要创造条件使用英语等外语进行公共课和专业课教学。

在文件精神指导下,全国普通高等学校尤其是重点高校中兴起了使用国外教材开展教学活动的潮流。如生物技术与工程、环境科学与工程、材料科学与工程及作为其学科基础理论重要组成部分的化学技术和化学工程技术又是这股潮流中最为活跃的领域之一。在教育部“化工类专业人才培养方案及教学内容体系改革的研究与实践”项目组及“化工类专业创新人才培养模式、教学内容、教学方法和教学改革的研究与实践”项目组和“全国本科化学工程与工艺专业教学指导委员会”的指导和支持下,化学工业出版社及时启动了引进国外名校名著的教材工程。

出版社组织编辑人员多次赴国外学习考察,通过国外出版研究机构对国外著名的高等学校进行调查研究,搜集了一大批国际知名院校的现用教材选题。他们还联络国内重点高校的专家学者组建了“国外名校名著评价委员会”,对国外和国内高等本科教学进行比较研究,对教材内容质量进行审查评议,然后决定是否引进。他们与国外许多著名的出版机构建立了联系,有的还建立了长期合作关系,以掌握世界范围内优秀教材的出版动态。

以其化学化工专业领域的优势资源为基础,化学工业出版社的教材引进主要涉及化学、化学工程与工艺、环境科学与工程、生物技术与工程、材料科学与工程、制药工程等专业,对过程装备与控制工程、自动化等传统专业教材的引进也在规划之中。

他们在影印、翻译出版国外教材的过程中,注意学习国外教材出版的经验,提高编辑素质,密切编读联系,整合课程体系,更新教材内容,科学设计版面,提高印装质量,更好地为教育服务。

在化工版“国外名校名著”系列教材即将问世之际,我们不仅感谢化学工业出版社为高等教育所做的努力,更应赞赏他们严谨认真的工作作风。

中国科学院院士,天津大学教授

余国琮

2002年8月

166005

To the memory of my parents, to Diane, and to Deborah and Benjamin

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

To my parents, Harry and Rebeca Lewin, to Ruti, and to Noa and Yonatan

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. Professor Hughes created comprehensive simulations of the decane chlorination process, on the cover, using FLOWTRAN.

About the Authors

Warren D. Seider is Professor of Chemical 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. Seider has contributed to the fields of process analysis, simulation, design, and control. He coauthored *FLOWTRAN Simulation—An Introduction* in 1974 and has coordinated the design course at Penn for nearly 20 years involving projects provided by many practicing engineers in the Philadelphia area. He has authored or coauthored over 70 journal articles and authored or edited six books. Seider was the recipient of the AIChE Computing in Chemical Engineering Award in 1992. He served as a Director of AIChE from 1984 to 1986 and has served as chairman of the CAST Division and the Publication Committee. He helped to organize the CACHE (Computer Aids for Chemical Engineering Education) Committee in 1969 and served as its chairman. Seider is a member of the Editorial Advisory Boards of *Industrial and Engineering Chemistry Research* and *Computers and Chemical Engineering*.

J. D. Seader is Professor of Chemical Engineering at the University of Utah. He received B.S. and M.S. degrees from the University of California at Berkeley and a Ph.D. from the University of Wisconsin. From 1952 to 1959, he designed processes for Chevron Research, and from 1959 to 1965, he conducted rocket engine research for Rocketdyne. Before joining the faculty at the University of Utah, Seader was a professor at the University of Idaho. He is the author or co-author of 102 technical articles, seven books, and four patents. Seader is co-author of the section on distillation in the 6th and 7th editions of *Perry's Chemical Engineers' Handbook*. He is coauthor of *Separation Process Principles*, published in 1998. Seader is Associate Editor of *Industrial and Engineering Chemistry Research*. He has been a trustee of CACHE for 27 years, serving as Executive Officer from 1980 to 1984. For 20 years, he directed the use by and distribution for universities of Monsanto's FLOWTRAN process simulation computer program. Seader served as a Director of AIChE from 1983 to 1985. In 1983, he presented the 35th Annual Institute Lecture of AIChE. In 1988, he received the Computing in Chemical Engineering Award of the CAST Division of AIChE.

Daniel R. Lewin is Associate Professor of Chemical Engineering at the Technion, the Israel Institute of Technology, situated overlooking Haifa Bay. He received his B. Sc. degree from the University of Edinburgh and his D. Sc. degree from the Technion. His research focuses on the interaction of process design and process control and operations, with emphasis on model-based methods. He has authored or co-authored over 60 research papers in the area of process systems engineering. Lewin has been awarded a number of prizes for research excellence. He received the Jacknow Award in recognition of teaching excellence at the Technion. He is currently serving as Associate Editor of the *Journal of Process Control* and is a member of International Federation of Automatic Control (IFAC) Committee on Process Control.

Preface

OBJECTIVES

A principal objective of this courseware is to describe modern strategies for the design of chemical processes. Since the early 1960s, the emphasis in undergraduate education has been on the engineering sciences. In recent years, however, more scientific approaches to 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 utilize the modern approaches to process design. Like workers in thermodynamics; momentum, heat, and mass transfer; and chemical reaction kinetics, process designers apply the principles of chemistry, physics, and biology. Designers, however, utilize these principles, and those established by engineering scientists, to create industrial chemical 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.

In this courseware, the latest design strategies are described, most of which have been improved significantly with the advent of computers, mathematical programming methods, and artificial intelligence. Since most curricula place little emphasis on 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 processes.

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 process creation, the use of flowsheet simulators to assist in process design, and the application of economics in venture analysis. To provide this instruction, the subject matter is presented in five parts, which describe the various aspects of process design. As discussed in Chapter 1, Figure 1.1 shows how these parts relate to the entire design process and to each other. All of the parts are presented at the senior level. To comprehend much of Part Four, "Plantwide Controllability Assessment," it is necessary to have completed a course in process control, as discussed below.

The emphasis throughout the text, and especially in Part One, on process invention, and Part Two, on process synthesis, is on the steps in process creation and the development of a base-case design(s). For the former, methods of tackling the primitive design problem, collecting data, and preparing the synthesis tree of alternative flowsheets are covered. Then, for the most promising flowsheets, a base-case design(s) is developed, including a detailed process flowsheet, with material and energy balances. The base-case design(s) then enters the detailed design stage, in which the equipment is sized, cost estimates are obtained, a profitability analysis is completed, and optimization is carried out, as discussed in Part Three.

Throughout this courseware, various methods are utilized to perform the extensive 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. Since the 1970s, many faculty have begun to augment the heuristic approach with an introduction to the analysis of prospective flowsheets using simulators, such as ASPEN PLUS, HYSYS, PRO-II, CHEM-

CAD, and FLOWTRAN. 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, has been to find the proper blend of modern computational approaches with simple heuristics.

In the early chapters, especially, emphasis is placed on the synthesis of conventional chemical processes, that is, processes that operate at steady state and present no unusual control problems. Even for these processes, the new dynamic simulators are useful for studying start-up, shut-down, upsets, and the performance of alternative control systems. Dynamic analysis often suggests designs that are easier to implement and control. As processes become more integrated, to achieve more economical operation, their responses to disturbances and setpoint changes become more closely related to the design integration, and consequently, the need to assess their controllability gains importance. To introduce several methods, Part Four is intended for readers who have studied linear control theory for single-input, single-output (SISO) controllers (usually in a first course in process control). Emphasis is placed on the methods for assessing the controllability of processes designed to operate at a steady state, with the consideration of frequency-dependent measures only when necessary. Controllers are designed for the most promising processes, and the ability of the processes to reject typical disturbances is evaluated using dynamic simulation. In summary, Part Four is intended to show that, to achieve more profitable designs, it is important to consider *plantwide control* during process design. This is accomplished using the simpler strategies for multiple-input, multiple-output (MIMO) control.

A further objective of this courseware is to illustrate the design strategies by applying them to 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 purification before streams are released into the environment. Several originate in the biochemicals industry, including fermentations to produce pharmaceuticals, foods, and chemicals. Others are involved in the manufacture of polymers and electronic materials. In addition to the processes interspersed throughout the chapters, 31 design-problem statements, prepared by industrial practitioners, are provided in Appendix VIII. For each problem statement, a process design has been completed by groups of two or three students at the University of Pennsylvania. See also the report, "Process Design Projects at Penn: 100 Problem Statements," edited by W.D. Seider and Arnold Kivnick, which was circulated to faculty members around the world in 1994.

FORMAT OF COURSEWARE AND THE MULTIMEDIA CD-ROM

For the most part, this courseware takes the form of a conventional textbook accompanied by computer programs to be utilized by the reader in various aspects of his or her design studies. As the design strategies have been elucidated during the development of this courseware, fewer and fewer specifics have been provided in the chapters concerning the software packages involved. Instead, Appendixes I–IV, VII, and IX have been developed to give many examples of the input and output and discuss in some detail the nature of the models provided for the processing units, with several example calculations presented as well. By far the most complete coverage is provided in the multimedia CD-ROM that accompanies the textbook. The CD-ROM uses voice, video, and animation to introduce new users of the steady-state simulators to the specifics of the systems, especially ASPEN PLUS and HYSYS. Approximately 50–60 hours of instructional materials are provided. These include several tutorials that provide instruction on the completion of input for ASPEN PLUS and HYSYS. During the next year, we plan to add coverage of CHEMCAD, and possibly PRO/II. In addition, video segments show portions of a petrochemical complex in operation, including distillation towers, heat exchangers, pumps and compressors, and chemical reactors. Murtaza Ali, Scott Winters, Diane M. Miller, Michael DiTillio, and Christopher S. Tanzi, at the University of Pennsylvania, have combined color photographs, animation, voice, and videotapes to enhance the instruction provided, with emphasis on ASPEN PLUS. D.R. Lewin, at the Technion, added the instructional materials on HYSYS.

The CD-ROM contains more than 500 Mb, and is packaged with each textbook. Included are files that contain the solutions for more than 60 examples using either ASPEN PLUS or HYSYS, as well as problems solved using DYNAPLUS and GAMS and the MATLAB scripts in Chapter 13. The files are referred to in each example and can easily be used to vary parameters and to explore alternative solutions. While it is planned to revise the textbook periodically, the CD-ROM will be revised annually. Furthermore, a Web site will be maintained at www.wiley.com/college/seider, in which revisions will be entered on a regular basis, especially as they relate to new releases of the commercial software.

ADVICE TO STUDENTS AND INSTRUCTORS

In the use of this textbook and CD-ROM, students and instructors are advised to take advantage of the following four features:

Feature 1

The textbook is organized around the key steps in process design shown in Figure 1.1. These steps reflect current practice and provide a sound sequence of instruction, yet with much flexibility in permitting the student and instructor to place emphasis on preferred subjects.

Students can study the chapters in Part One in sequence. Although they provide many examples and exercises, the appendices and CD-ROM can be referred to for details of the process simulators. Chapters in Parts Two, Three, and Four can be studied as needed. There are many cross-references throughout the text—especially to reference materials needed when carrying out designs. For example, students can begin to learn heuristics for heat integration in Chapter 2, learn algorithmic methods in Chapter 7, learn the strategies for designing heat exchangers and estimating their costs in Part Three (Chapters 8 and 9), and learn the importance of examining the controllability of heat-exchanger networks in Part Four.

Instructors can begin with Part One and design their courses to cover the other chapters as desired. Because each group of students has a somewhat different background depending on the subjects covered in prior courses, the textbook is organized to give instructors much flexibility in their choice of subject matter and the sequence in which it is covered. Furthermore, design instructors often have difficulty deciding on a subset of the many subjects to be covered. This book provides sufficiently broad coverage to permit the instructor to emphasize certain subjects in lectures and homework assignments, leaving others as reference materials to be used by the students when carrying out their design projects. In a typical situation, when teaching the students to generate design alternatives, select a base-case design, and carry out its analysis, the textbook enables the instructor to place emphasis on one or more of the following subjects: synthesis of separation trains (Chapter 5), energy efficiency (lost work analysis and heat and power integration—Chapters 6 and 7), process unit design (e.g., heat exchangers—Chapter 8), and controllability assessment (Part Four).

Feature 2

Process synthesis is introduced mostly using heuristics in Part One (Chapters 2 and 4), whereas Part Two provides more detailed algorithmic methods for separation train synthesis and heat and power integration.

This feature enables the student to begin carrying out process designs using easy to understand rules of thumb when studying Part One. As these ideas are mastered, the student can learn algorithmic approaches that enable him or her to produce better designs. For example, Chapter 2 introduces two alternative sequences for the separation of a three component mixture (in the vinyl chloride process), whereas Chapter 5 shows how to generate and evaluate many alternatives for the separation of multicomponent mixtures, both ideal and nonideal.

This organization provides the instructor the flexibility to emphasize those subjects most useful for his or her students. Part One can be covered fairly quickly, giving the students enough background to begin work on a design project. This can be important at schools where only one semester is allotted for the design course. Then, as the students are working on their design projects, the instructor can take up more systematic, algorithmic methods, which can be applied to improve their designs. In a typical situation, when covering Part One, the instructor would not cover nonideal separations, such as azeotropic, extractive, or reactive distillations. Consequently, most students would begin to create simple designs involving reactors followed by separation trains. After the instructor covers the subject matter in Chapter 5, the students would begin to take advantage of more advanced designs.

Feature 3

Process simulators, both steady state and dynamic, are used throughout the textbook (ASPEN PLUS, HYSYS, CHEMCAD, PRO/II, and DYNAPLUS). This permits access to large physical property, equipment, and cost data bases and the examination of aspects of more than 20 chemical processes. Emphasis is placed on the usage of simulators to obtain data and perform routine calculations throughout.

Through the use of the process simulators, students learn how easy it is to obtain data and perform routine calculations. They learn effective approaches to building up knowledge about a process through simulation. The appendices and CD-ROM provide the students with 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 data base and to perform routine calculations, when computing heat loads, heats of reaction, and vapor/liquid equilibria. Then, in Chapter 3, two examples show how to use the simulators to assist in the synthesis of toluene hydrodealkylation and monochlorobenzene separation processes. Virtually all 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 CD-ROM contain so many routine examples of how the simulators are useful in building up a process design, the instructor has time to emphasize other aspects of process design. Through the examples and multimedia instruction on the CD-ROM, the students obtain the details they need to use the simulators effectively, saving the instructor class time, as well as time answering detailed questions as the students prepare their designs. Consequently, the 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 and CD-ROM 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, they create a separation section and eventually add recycle. Thanks to the coverage of the process simulators in Part One, the appendixes, and the CD-ROM, the instructor would review only the highlights in class.

Feature 4

To our knowledge, this design book is the first to emphasize the importance of assessing plantwide controllability. Modern computing tools are enabling practitioners and students to be more aware that processes selected on the basis of steady-state economics alone often perform poorly and are less profitable.

When studying Chapter 12, students learn that they can begin to screen processes during process synthesis by selecting the variables to be measured and adjusted and beginning to formulate control loops, but *without* detailed controller design. Then, in Chapter 13, well-established methods enable students to screen alternative processes using standard linear approximations, again *without* detailed controller design. Finally, in Chapter 14, for

the most promising processes, the controllers are designed and simulations are carried out to show that the analyses in Chapter 13 are effective. Throughout Part Four (Chapters 12–14), alternatives for heat-exchanger networks; heat-integrated distillation towers; stirred-tank reactor designs; and processes with reactors, separators, and recycle loops are compared to show that there are significant differences in controllability and resiliency.

From the instructor's perspective, although it is widely recognized that this subject needs to be addressed, most have not had access to sufficiently good teaching materials and computing systems to provide adequate coverage. In Chapter 12, basic introductory material is provided that can be taught with little effort. Chapter 13 is more advanced. Although some instructors will cover it thoroughly, others may prefer to select from among the case studies to introduce their students to the effectiveness of controllability and resiliency analysis for linearized systems. Then, even if time is not available for the students to tune controllers and run dynamic simulations, Chapter 14 can be used to show the effectiveness of this approach during process design. In a typical situation, the instructor would use the alternative heat-exchanger networks, heat-integrated distillation towers, reactor sequences, and/or processes with recycle to show the importance of considering controllability in the design process.

ONE- OR TWO-SEMESTER COURSES

In one semester, it is possible to cover Part One, many topics in Part Two, and Chapters 8, 9, 10, and 12. Students solve homework exercises and take midsemester and final exams but do not work on a comprehensive design project. The latter is reserved for a design project course in a second semester. Alternatively, many departments teach design concepts in a single course, which includes a comprehensive design project. For such a course, the same materials can be covered, somewhat less thoroughly, or a subset of the subjects can be covered. The latter often applies in departments that cover design-related topics in other courses. For example, many departments teach economic analysis before the students take a process design course. Other departments teach the details of heat-exchanger design in the heat-transfer course. This courseware is well suited for these courses because it provides much reference material that can be covered as needed.

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Senior students at the University of Pennsylvania, Murtaza Ali, Scott Winters, Diane M. Miller, Michael DiTillio, and Christopher S. Tanzi, implemented the multimedia CD-ROM and assisted in many other ways. Their efforts are also appreciated. In this regard, seed money for development of the CD-ROM was provided by Dean Gregory Farrington, University of Pennsylvania, and is acknowledged gratefully.

Several colleagues at the University of Pennsylvania and industrial consultants from local industry in the Philadelphia area were very helpful as these materials evolved, especially Arnold Kivnick, Robert M. Busche (Bio-en-gene-er Associates, Wilmington, DE), F. Miles Julian, and Robert F. Hoffman. Arnold has worked with senior design teams each year since 1956, more recently as adjunct professor. He critiqued many sections of

this textbook. Bob Busche served as adjunct professor for 13 years, in which he presented lectures and course notes entitled "Venture Analysis: A Framework for Venture Planning," which served as the basis for Chapters 9 and 10. He also provided many excellent design projects in the biochemicals area, several of which appear in Appendix VIII. Miles critiqued Chapters 9 and 10 and provided many excellent design projects.

Much assistance was provided by four colleagues at ARCO Chemical Company: Leonard A. Fabiano, David Kolesar, Robert A. Knudsen, and Robert Nedwick, who have provided excellent design projects and assistance to our student design teams since the late 1970s, who spent considerable time critiquing the chapters of this textbook, and who helped us to better utilize the features of ASPEN PLUS. Their contributions have been especially helpful. The assistance of Robert Maxwell and Winston Lewis, also of ARCO, is very much appreciated.

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As this courseware approached the publication stage, A. Wayne Anderson, the College Publisher at John Wiley & Sons, responded enthusiastically. Wayne's excellent advice and guidance throughout the publication of this courseware is very much appreciated.

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W.D. Seider
J.D. Seader
D.R. Lewin
April 1998

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