Coordinating Equilibrium-based and Rate-based Separations Courses with the Senior Process Design Course

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The undergraduate education of a chemical engineer has, for more than half a century, included a senior course in design. In early years, as exemplified in the textbook, Chemical Engineering Plant Design", by Vilbrandt[1], emphasis was placed not on process design, i.e. design of the process structure and the equipment, but on plant design, including consideration of foundations, drainage, piping installation, buildings, power transmission, plant location, plant layout, and preconstruction cost estimates. Some attention was given to selection and arrangement of equipment. The textbook, "Plant Design and Economics for Chemical Engineers", which first appeared in 1958 and now, under the authorship of Peters and Timmerhaus[2] is in its fourth edition, took a much different approach, greatly emphasizing the economic aspects of plant design, including cost estimation and profitability analysis. In addition, extensive chapters were provided on design and costing of equipment for materials transfer and handling, heat transfer, mass transfer, and chemical reactions. In Peters and Timmerhaus, emphasis shifted from plant design to process design, but little attention was given to the synthesis of a process structure.

Prior to the 1960s, the development, by practicing chemical engineers in industry, of a process design for a given process structure, including material and energy balances and overall sizing of equipment, was carried out by hand calculations, which were often tedious and sometimes lacking in rigor and accuracy. The textbooks by Vilbrandt and, especially, by Peters and Timmerhaus were adequate for teaching plant or process design conducted in this manner. Courses taken as prerequisites for the senior design course provided the necessary skills to conduct material and energy balance calculations and to determine equipment sizes, based on accepted practice at that time. However, the advent of large digital computers and the FORTRAN language in the mid 1950s provided a means to change significantly the process design procedure.

In 1958, the first evidence of the application of digital computers to perform material and energy balance calculations for complex chemical processes was reported in an article by Kessler and

Kessler[3]. In the 1960s, it was known that several large companies, including Chevron, duPont, EXXON, Monsanto, Shell, and Union Carbide were developing computer-aided process design programs. By 1967, as reported by Evans, Steward, and Sprague[4], six commercial computer-aided process design programs for steady-state operation, all written in FORTRAN, were referenced in the literature. It was believed at that time that all large companies in the petroleum industry and most large chemical companies were using computer-aided process design programs.

During the same period from the mid 1950s to the late 1960s, computers were also spurring revolutions in (1) computational procedures for physical equilibrium, chemical equilibrium, and multiple equilibrium-stage separation operations for multicomponent mixtures, and (2) correlations for thermodynamic properties, especially fugacities, activity coefficients, enthalpies, and enthalpies. Both of these developments had the potential to greatly increase the accuracy of process design.

Prior to the 1950s, stage and reflux requirements for multicomponent distillation were determined by (1) graphical pseudo-binary methods using McCabe-Thiele or Ponchon-Savarit diagrams, (2) the shortcut procedure of Fenske, Underwood, and Gilliland, or (3) very tedious and iterative stage-to-stage calculations, one equation at a time, using the Lewis-Matheson or Thiele-Geddes methods. In fact, almost all of chemical engineering calculations were made by solving one equation at a time. In 1957, the leading textbook on applied mathematics for chemical engineers, by Mickley, Sherwood, and Reed[5], did not discuss matrix algebra. The importance of matrices to chemical engineering, especially for multicomponent, multistage calculations, was first espoused by Acrivos and Amundson[6] in 1955. This was followed in 1958 by an article by Amundson and Pontinen[7], who solved the material balance and equilibrium equations for all stages simultaneously for each component, using matrix algebra methods. In 1962, Lapidus[8] emphasized matrices in his numerical mathematics book for chemical engineers, and in 1966, Amundson[9] completed an entire textbook on the application of matrices to chemical engineering. Today, computer-aided process design programs make extensive use of matrix algebra in solving mathematical models for process equipment.

Prior to the 1960s, K-values and enthalpies of hydrocarbons for vapor-liquid equilibrium calculations were determined almost exclusively by charts, such as those of DePriester[10], and those in the 1957 "Equilibrium Ratio Data Book" of the Natural Gasoline Association of America in Tulsa, OK. For chemical mixtures that form non-ideal liquid solutions, K-values were computed from a modified Raoult's law using vapor pressure data and relatively simple liquid-phase activity coefficient equations, such as those of van Laar and Margules. The first accurate equation-of-state method for predicting thermodynamic properties of hydrocarbons, that of Benedict, Webb, and Rubin[11], had appeared in 1951, but it was very complex and not suitable for hand calculations.

With the advent of computers in the late 1950s, complex equations for predicting thermodynamic properties could now be justified and, as the equations were developed, they were rapidly incorporated into computer-aided process design programs. These computer methods include (1) equation-of-state methods, most notably Soave-Redlich-Kwong and Peng-Robinson, and (2) liquid-phase activity-coefficient methods, most notably Wilson, NRTL, UNIQUAC, and

UNIFAC. Initially, use of equation-of-state methods was restricted to hydrocarbon and light gas mixtures. However, recent advances in the formulation of mixing rules, e.g. by Wong and Sandler[12], are permitting applications to mixtures containing polar organic molecules as well.

The important result of all this effort in thermodynamics and mathematical modeling with numerical methods is that computer-aided process design can be accomplished rapidly and more accurately than by pre-computer hand-calculation methods. Furthermore, the emergence of very fast and inexpensive personal computers with large memory has given every practicing chemical engineer easy access to such methods. Computer-aided process design has been wholeheartedly embraced by the chemical process industries. Whereas, in the 1960s and 1970s large companies developed their own in-house computer-aided process design programs (called process simulators), today all companies, large and small can license the use of such programs from simulation companies.

The incorporation of process simulation into the undergraduate curriculum in chemical engineering was slow to develop and lagged behind industrial use. The first organized attempt to make process simulation available to instructors in chemical engineering was that of Professor Paul T. Shannon at Purdue University, who, in 1967, made his PACER program available. In 1971, Shannon[12], together with five other professors, all from McMaster University, published the first book on simulation. PACER lacked a physical property estimation package, which limited its usefulness. This was remedied in 1968 by the CHESS program of Professors R. L. Motard and E. J. Henley. However, their program, as well as PACER, lacked a general, rigorous, multistage, multicomponent separation model for distillation-type operations.

In 1974, the CACHE (Computer Aids for Chemical Engineering Education) Committee, which had been formed in 1969, announced the availability of the Monsanto process simulator, FLOWTRAN, to educators via a network. FLOWTRAN was an advanced commercial process simulator, complete with an extensive set of equipment and physical property models. In 1982, Monsanto agreed to allow departments of chemical engineering to install FLOWTRAN on their own computers, thus greatly facilitating its use by students and instructors. The introduction of FLOWTRAN into educational use was accompanied in 1974 by a textbook by Seader, Seider, and Pauls[13]. By 1993, three editions of that text had been published, and the program had been installed by 141 departments in the United States, 11 in Canada, 38 in 21 other countries.

In the 1980s and 1990s, Monsanto, like other companies, curtailed and eventually discontinued development of its in-house simulator as process simulation companies, such as AEA Technology, Aspen Technology, ChemShare, Chemstations, and Simulation Sciences began to offer process simulators for license. These simulation companies also offered the use of their programs, at very low fees or at no cost, to universities for instructional purposes. In 1994, the use of FLOWTRAN by universities had been largely replaced by the use of ASPEN PLUS, ChemCAD, HYSIM, and PRO/II. Accordingly, Monsanto discontinued licensing FLOWTRAN. Today, almost all departments of chemical engineering include, in the senior design course, instruction in the use of one of the four commercial process simulators.

Computed-aided process design makes use of mathematical procedures that were not utilized in pre-computer methods of design. Many of these methods had been developed by the late 1970s

and they were presented by Westerberg, Hutchison, Motard, and Winter[14], in 1979, in a very useful textbook, entitled "Process Flowsheeting". Topics in that book included solving linear and nonlinear equations, computerized physical property systems, degrees of freedom in a flowsheet, the sequential modular approach to simulation, convergence of recycle, and design specifications. Because intelligent use of process simulators required knowledge of these topics, some instructors began to include them in the senior design course.

A prerequisite for the use of a process simulator is a process flow diagram, in which the equipment and its arrangement is given. That is, the use of a process simulator presupposes completion of the process synthesis step. In the early 1970s, computer-aided techniques for process synthesis began to emerge. Methods for synthesizing heat exchanger networks to minimize energy usage are now well developed and are now taught in many senior design courses. The sequencing of separation systems has also received much attention and is also taught to seniors. More difficult has been the development of systematic methods for synthesizing reactor networks and entire processes.

The third edition, in 1980, of the design textbook by Peters and Timmerhaus included a brief mention of computer-aided design, but no formal instruction and no mention of process synthesis. The 1991 fourth edition added a short chapter on computer-aided design, including some aspects of process synthesis. Considerably more emphasis was given to process synthesis in the 1988 textbook by Douglas[15], which also included a short chapter on computer-aided design programs, with emphasis on FLOWTRAN, but stressed the importance of shortcut design methods in the early stages of design. A similar approach to process design is taken by Smith[16] in a 1995 textbook, except that no mention is made computer-aided design or process simulators.

Judging by the material covered in the above-mentioned design textbooks, as well as two other very recent books by Biegler, Grossmann, and Westerberg[17], and by Turton, Bailie, Whiting , and Shaelwitz[18], it appears that the following approaches are being used to teach the senior design course:

1. Emphasis on economics, and sizing and costing of equipment, as in Peters and Timmerhaus.

2. Emphasis on the development of the flowsheet, as in Douglas, and in Smith.

3. Emphasis on systematic methods of process synthesis, and development of mathematical models for simulation and optimization., as in Biegler, Grossmann, and Westerberg.

4. Emphasis on synthesis, design, and performance of processes, as in Turton, Bailie, Whiting, and Shaeiwitz.

Regardless of the approach taken, all senior design courses culminate with a design project. Some instructors assign the annual National Student Design Competition problem of the AIChE, which can be worked on an individual or group basis. In some cases, the students are not required to adhere to the contest rules. Other instructors, particularly those whose universities are located near chemical plants, enlist the aid of industrial consultants experienced in process design, who propose a process design problem and supervise students in the development of a

design and economic evaluation, as discussed by Seider and Kivnick[19]. Still other instructors, particularly those with industrial experience, develop their own design problems and supervise the development of student solutions. Those using the AIChE contest problem have witnessed some significant changes during the past few years. Until 1995, students were required, under contest rules, to work on the problem individually. Now, they can work as individuals or as teams of two or three students. Starting in the 1997 contest problem, specific mention was made of the use of process simulators to obtain an optimal design. In fact, the 1997 and 1998 contest problems were best solved by a process simulator because of the number of components involved, the need for recycle, the need to purge, and the complex nature of the separation systems.

While a revolution has occurred in the structure of the senior design course, particularly with respect to (1) the shift from plant design to process design, (2) the addition of techniques for synthesizing a process, and (3) the use of a process simulator to perform mass balances, energy balances, and equipment sizing, using complex property and equipment models, little seems to have changed in the way that separations courses are taught. At most schools, the main topics are still (1) absorption and stripping of dilute solutions using graphical methods or the Kremser equation, (2) binary distillation by the McCabe-Thiele and Ponchon-Savarit graphical methods, (3) ternary liquid-liquid extraction by the Hunter-Nash triangular graph or Varteressian-Fenske auxiliary distribution diagram methods. These methods date back to the period from 1921 to 1936, more than 60 years ago. The virtue of these methods lies in the ability to visualize what is happening and to quickly observe the effects of the variables. Thus, despite their lack of rigor or difficulty in obtaining an accurate solution, they continue to be popular, and justifiably so. Nevertheless, it appears that the majority of undergraduate students are not being prepared adequately to utilize the enormous power and versatility of the separation models in process simulators.

In 1986, R. Byron Bird[20], in a tribute to Olaf A. Hougen, who died that year, cited some guideposts for chemical engineering departments. Included was the statement, "There should be a smooth flow of information from graduate research to undergraduate teaching". Graduate instruction in an area can put pressure for modernization on the undergraduate course in the same area. But changes in the undergraduate course should come only after careful testing at the graduate level. That testing has been adequately carried out for the multicomponent, multistage separation models in process simulators. The following is an example of how the contents of the junior-year separations (equilibrium stage and mass transfer) course(s) can be coordinated with the senior design course(s) to enable chemical engineering graduates at the B.S. level to make significant contributions in the workplace. It presupposes that prior to the separations course(s), the student completes a solution thermodynamics course that covers modern methods of determining multicomponent phase equilibria

In the summer of 1998, a new process design textbook by Seider, Seader, and Lewin[21], entitled, "Process Design Principles: Synthesis, Analysis, and Evaluation", will be published by John Wiley & Sons. The table of contents of this textbook is shown in Table 1. The most important objective of the textbook is to describe the strategies and approaches for the design of chemical processes. The process designer, utilizes principles learned in thermodynamics; momentum, heat and mass transfer; chemical reaction kinetics; and process control, together with the

fundamentals of chemistry, physics, and mathematics. To these are added principles of process engineering and economics to create safe, efficient, controllable, and economical industrial chemical processes that satisfy societal needs while returning a profit. In so doing, the designer emphasizes methods of process synthesis and optimization in the face of uncertainties, often utilizing the results of analysis and experimentation prepared in cooperation with engineering scientists.

The textbook describes the latest design strategies, most of which have been improved significantly with the advent of computers, mathematical programming methods, and artificial intelligence. Since most chemical engineering curricula place little emphasis on design strategies prior to design courses, the textbook and accompanying CD-ROM is intended to provide a smooth transition for students and engineers that are called upon to design creative new processes. As seen in Table 1, the subject matter is presented in five related parts, which describe the various aspects of process design. To comprehend much of Part IV, Plant-wide Controllability Assessment, it is necessary to have completed a course in process control.

The emphasis throughout the text, and especially in Parts I, process invention, and II, 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. As discussed in Part III, 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 Chapter 11.

Throughout the text, 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 the text and the accompanying CD-ROM. We believe, based on our experience, that for senior students, this approach is preferred over the 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.

Over the past 20 years, many faculty have begun to augment the heuristic approach to design with an introduction to the analysis of prospective flowsheets using simulators, such as ASPEN PLUS, ChemCAD, ChemShare, FLOWTRAN, HYSIM, and PRO/II. Today, most schools use one of these simulators, but often without adequate teaching materials. Consequently, the challenge for us, in the preparation of the our new process design textbook, has been to find the proper blend of modem computational approaches with simple heuristics.

As seen in Table 1, 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, new dynamic simulators, like DYNAPLUS, HYSYS, and SPEEDUP, are useful for studying startup, shutdown, 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 IV is intended for readers who have studied linear control theory for single-input, single-output (SISO) controllers (usually in the first course in process control). Emphasis is placed on 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 are evaluated using dynamic simulation. In summary, Part IV is intended to show that to achieve more profitable designs it is important to consider plant-wide control during process design. This is accomplished using the simpler strategies for multiple-input, multiple-output (MIMO) control.

A further objective of our new process design textbook is to illustrate design strategies by applying them to chemical processes in several industries. Many are derived from the petrochemical industry, with emphasis on environment 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 biochemical industry, including fermentation 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 during the past two decades.

Although, we believe strongly in the use of a process simulator throughout the course, much of the instruction for their use is provided in Appendices I-IV, as seen in Table 1. These appendices, which are referenced in the chapters, give many examples of computer 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. However, by far, the most complete coverage is provided in the multi-media CD-ROM that accompanies the textbook. The CD-ROM uses voice, video, and animation to introduce new users of steady-state simulators to the specifics of the systems, especially for ASPEN PLUS and HYSYS. Several tutorials provide instruction on the completion of input for ASPEN PLUS and HYSYS. In addition, video segments show portions of a petrochemical complex in operation including distillation towers, heat exchangers, pumps and compressors, and chemical reactors. Over the past four years, Murtaza Ali, Scott Winters, Diane Miller, and Michael DiTillio, four Seniors in chemical engineering at the University of Pennsylvania, have combined color photographs, animation,. voice, and video tapes to enhance the instruction provided. The CD-ROM contains approximately 400 Mb, and will be packaged with each textbook. Included are files that contain the solutions of over 60 examples using either ASPEN PLUS or HYSYS. The files are referred to in each example and can easily be used to vary parameters and to explore alternative solutions.

Current process simulators include rigorous multicomponent, multistage equilbrium models that utilize the most rigorous models for computing thermodynamic properties, particularly those for phase equilibria. Furthermore, the equilibrium models can be applied to complex configurations, including multiple feeds, sidestreams, phase splitting, simultaneous chemical reaction, and handling of azeotropes. However, experience has shown that students need to receive instruction

in the formulation and application of these models so that their possibilities are clear and their application can be carried out with a minimum of failures. Ideally, such instruction should precede the senior design course. The logical place for the material is the junior courses in separations, equilibrium-stage operations, mass transfer, and/or rate-based separations.

In 1963, E. J. Henley and H. K. Staffin authored a book entitled, “Stagewise Process Design”, which introduced chemical engineering students to non-diffusional aspects of material and energy balances under phase equilibria constraints, using mainly graphical methods. Most of that book was incorporated, in 1981, into a much expanded textbook, “Equilibrium-Stage Separation Operations in Chemical Engineering” by E. J. Henley and J. D. Seader. The objective of the 1981 book was to add, to the 1963 book, material on the mathematics and science associated with multicomponent, multistaged calculations as implemented in commercial, steady-state process simulation computer programs, which were becoming widely available and which relied on numeric, rather than graphical, methods of solution. These programs are relatively easy to use, but to avoid convergence problems and impossible specifications, the user must have a firm understanding of the fundamentals of chemical engineering. The 1981 textbook, hopefully, provided that understanding.

Since publication of the Henley and Seader textbook, interest in the design and simulation of separation operations using mass-transfer (rate-based) principles has increased considerably. This has been due to the availability of improved packings for packed columns used in absorption, distillation, and stripping; and to the development of theory and applications for the less mature separation operations of adsorption, crystallization, and membrane separations. During the same period, batch distillation, for which rigorous, computer-based calculation methods have been developed, has found wider application. Also, greatly improved procedures for the development of separation processes using enhanced distillation (azeotropic, extractive, pressure-swing, and reactive) have been published, and new applications of supercritical-fluid extraction and chromatography have been commercialized. The 1981 textbook contained little material on these topics. A new textbook by Seader and Henley[22], entitled "Separation Process Principles" was published early in 1998. In this new textbook, substantial material is presented on both equilibrium-based and rate-based methods.

The table of contents for Seader and Henley is given in Table 2. As seen, the textbook is divided into three parts. Part I, which consists of five chapters, presents introductory concepts. In Chapter 1, the many ways in which chemical mixtures are separated industrially are described. Chapter 2 is a review of solution thermodynamics, for both equilibrium-based and rate-based approaches to separation operations. This chapter can be omitted and just used for reference if students have completed or are taking concurrently a course in chemical engineering thermodynamics. Chapter 3 covers the basic principles of diffusion and mass transfer required for the rate-based approach to separation operations. The use of phase equilibrium and material balance equations to solve a wide range of single equilibrium stage separations is covered in Chapter 4, while Chapter 5 introduces the student to multiple, equilbrium cascades, with emphasis on countercurrent flow of the two phases being contacted.

The remaining two parts of the textbook are organized as to the method of separation. In Part II, separations achieved by phase creation or addition are presented. Chapters 6 through 8 cover

classical graphical and algebraic methods for absorption and stripping of dilute solutions, binary distillation, and ternary liquid-liquid extraction. Chapters 9 through 12 cover theory and applications of all the computer-based methods used in simulation programs for vapor-liquid and liquid-liquid separations. Included in Chapter 9 is the important Fenske-Underwood-Gilliland method for the preliminary determination of stage and reflux requirements for distillation, and the Kremser algebraic method for the preliminary determination of solvent and stage requirements for absorption, stripping, and extraction. The rigorous multicomponent, multistage equilibrium-based algorithms widely used in process simulators are presented in considerable detail in Chapter 10. The treatment includes the Newton simultaneous correction method and the inside-out method. The intelligent application of these methods to enhanced distillation, utilizing triangular diagrams where possible, is covered in detail in Chapter 11. Theory and application of the new mass-and-heat transfer-based methods for multicomponent, multistage separations that are used in the ChemSep program and the RATEFRAC program of ASPEN PLUS is presented in Chapter 12. Chapter 13 presents all of the methods used in process simulators to compute multicomponent, multistage batch distillation.

Separations by barriers and solid agents are presented in Part III, with membrane separations in Chapter 14, and adsorption, ion exchange, and chromatography in Chapter 15. Membrane separators have not yet been added to the equipment model libraries of process simulators. The SPEEDUP program of Aspen Technology, in conjunction with the ADSIM program, does compute fixed-bed adsorption.

It is suggested that instructors who teach the junior course(s) in separations, equilibrium-stage operations, rate-based operations, and/or mass transfer consider including the type of material presented in Chapters 9 through 15 of Seader and Henley. This can be done by reducing the amount of instruction on graphical methods for two- and three-component systems. This should prepare students, when using process simulators, to tackle more difficult design problems, which seem to be the norm, judging by the problem statements of recent AIChE student contest problems. Certainly, the use of a process simulator does make it possible to tackle, in a creative fashion, far more difficult design problems than in the past.

Table 1
Contents of Seider, Seader, and Lewin

Part I Process Invention - Heuristics and Analysis

Chap. 1: The Design Process

Chap. 2: Process Creation
Chap. 3: Simulation to Assist in Process Creation
Chap. 4: Heuristics for Process Synthesis

Part II Detailed Process Synthesis - Algorithmic methods

Chap. 5: Synthesis of Separation Trains
Chap. 6: Second-Law Analysis
Chap. 7: Heat and Power Integration

Part III Detailed Design, Equipment Sizing, Economics and Optimization

Chap. 8: Heat Exchanger Design

Chap. 9: Capital Cost Estimation
Chap. 10: Profitability Analysis
Chap. 11: Optimization of Process Flowsheets

Part IV Plant-wide Controllability Assessment

Chap. 12: The Interaction of Process Design and Process Control
Chap. 13: Flowsheet Controllability Analysis
Chap. 14: Dynamic Simulation of Processes

Part V Design Report

Chap. 15: Written Design Report and Oral Presentation

Appendices

I: ASPEN PLUS in Process Design
II: HYSYS in Process Design
III: Phase Equilibria and Unit Operation Models

IV: Physical Property Estimation, Solids Handling and Electrolytes
V: Residue Curves for Heterogeneous Systems
VI: Successive Quadratic Programming
VII: General Algebraic Modeling Systems

VIII: Design Problem Statements
IX: Dynamic Simulation Using DYNAPLUS
X: Heuristics for Process Equipment Design

XI: Materials of Construction
XII: Generation of Linear Models

Multi-media CD-ROM

"Steady-state Simulation of Process Flowsheets" by W. D. Seider, M. Ali, S. Winters, D. Miller, & M. DiTillio

Table 2
Contents of Seader and Henley

Part I: Introductory Concepts

Chapter 1: Separation Processes
Chapter 2: Thermodynamics of Separation Operations
Chapter 3: Mass Transfer and Diffusion
Chapter 4: Single Equilibrium Stages and Flash Calculations
Chapter 5: Cascades

PART II: Separation by Phase Creation or Addition

Chapter 6: Absorption and Stripping of Dilute Mixtures
Chapter 7: Distillation of Binary Mixtures
Chapter 8: Liquid-Liquid Extraction with Ternary Systems
Chapter 9: Approximate Methods for Multicomponent, Multistage Separation
Chapter 10: Equilibrium-Based Methods for Multicomponent Absorption, Distillation, and Extraction
Chapter 11: Enhanced Distillation and Supercritical Extraction
Chapter 12: Rate-Based Models for Distillation
Chapter 13: Batch Distillation

PART III: Separation by Barriers and Solid Agents

Chapter 14: Membrane Separations
Chapter 15: Adsorption, Ion Exchange, and Chromatography

References

1. Vilbrandt, F. C., "Chemical Engineering Plant Design", Third Edition, McGraw-Hill Book Company, Inc., New York, NY (1949). First edition published in 1934.

2. Peters, M. S., and K. D. Timmerhaus, "Plant Design and Economics for Chemical Engineers", Fourth Edition, McGraw-Hill Book Company, Inc., New York, NY (1958). First edition by Peters in 1958.

3. Kesler, M. G., and M. M. Kessler, "Engineering a Process with a Computer", World Petroleum, 29 (8) 60-63 (1958).

4. Evans, L. B., D. G. Steward, and C. R. Sprague, "Computer-Aided Chemical Process Design", Chem. Eng. Progress, 64 (4) 39-46 (1968).

5. Mickley, H. S., Sherwood, T. K., and C. E. Reed, "Applied Mathematics in Chemical Engineering", Second Edition, McGraw-Hill Book Company, Inc., New York, NY (1957).

6. Acrivos, A., and N. R. Amundson, "Applications of Matrix Mathematics to Chemical Engineering Problems", Ind. Eng. Chem., 47, 1533-1541 (1955).

7. Amundson, N. R., and A. J. Pontinen, "Multicomponent Distillation Calculations on a Large Digital Computer, Ind. Eng. Chem., 50, 730-736 (1958).

8. Lapidus, L., "Digital Computation for Chemical Engineers", McGraw-Hill Book Company, Inc., New York, NY (1962).

9. Amundson, N. R., "Mathematical Methods in Chemical Engineering - Matrices and Their Application", Prentice-Hall, Inc., Eaglewood Cliffs, NJ (1966).

10. DePriester, C. L., Chem. Eng. Progr., Symp. Ser., **49** (7) 1 (1953).

11. Wong, D. S. H., and S. I. Sandler, "A Theoretically Correct Mixing Rule for Cubic Equations of State", AIChE Journal, 38, 671-680 (1992).

12. Crowe, C. M., A. E. Hamielec, T. W. Hoffman, A. I. Johnson, D. R. Woods, and P. T. Shannon, "Chemical Plant Simulation - An Introduction to Computer-Aided Steady-State Process Analysis", Prentice-Hall, Inc., Englewood Cliffs, NJ (1971).

13. Seader, J. D., W. D. Seider, and A. C. Pauls, "FLOWTRAN Simulation - An Introduction", CACHE Corp., Austin, TX (1974).

14. Westerberg, A. W., H. P. Hutchison, R. L. Motard, and P. Winter, "Process Flowsheeting", Cambridge University Press, Cambridge, United Kingdom (1979).

15. Douglas, J. M., "Conceptual Design of Chemical Processes", McGraw-Hill Book Company, New York, NY (1988).

16. Smith, R., "Chemical Process Design", McGraw-Hill Book Company, New York, NY (1995).

17. Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, "Systematic Methods of Chemical Process Design", Prentice-Hall, Inc., Upper S

ddle River, NJ (1997).

18. Turton, R., R. C. Bailie, W. B. Whiting, and J. A. Shaeiwitz, "Analysis, Synthesis, and Design of Chemical Processes", Prentice-Hall, Inc., Upper Saddle River, NJ (1998).

19. Seider, W. D., and A. Kivnick, "Process Design Curriculum at Penn - Adapting for the 1990s", Chem Eng. Education, 28 (2) 92-97 (1994).

20. Bird, R. B., "Hougen's Principles", Chem. Eng. Education, 20 (4) 161-163 (1986).

21. Seider, W. D., J. D. Seader, and D. R. Lewin, "Process Design Principles: Synthesis, Analysis, and Evaluation", John Wiley & Sons, Inc., New York, NY (1998).

22. Seader, J. D., and E. J. Henley, "Separation Process Principles", John Wiley & Sons, Inc., New York, NY (1998).