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H. Scott Fogler

Elements of Chemical Reaction Engineering

Third Edition

Prentice Hall International Series
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Elements of Chemical Reaction Engineering

Third Edition

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Preface

"The man who has ceased to learn ought not to be allowed to wander around loose in these dangerous days."

M. M. Coady
(ca. 1870)

A. The Audience

This book is intended for use as both an undergraduate- and graduate-level text in chemical reaction engineering. The level of difficulty will depend on the choice of chapters to be covered and the type and degree of difficulty of problems assigned. Most problems requiring significant numerical computations can be solved with a personal computer using either POLYMATH or MATLAB.

B. The Goals

B.1. To Develop a Fundamental Understanding of Reaction Engineering

The first goal of this book is to enable the reader to develop a clear understanding of the fundamentals of chemical reaction engineering. This goal will be achieved by presenting a structure that allows the reader to solve reaction engineering problems through reasoning rather than through memorization and recall of numerous equations and the restrictions and conditions under which each equation applies. To accomplish this, we use (1) conventional problems that reinforce the student's understanding of the basic concepts and principles (included at the end of each chapter); (2) problems whose solution requires reading the literature, handbooks, or other textbooks on chemical engineering kinetics; and (3) problems that give students practice in problem

definition and alternative pathways to solutions. The algorithms presented in the text for reactor design provide a framework through which one can develop confidence through reasoning rather than memorization.

To give a reference point as to the level of understanding required in the profession, a number of reaction engineering problems from the *California Board of Registration for Civil and Professional Engineers—Chemical Engineering Examinations* (PECEE) are included. Typically, each problem should require approximately one-half hour to solve. Hints on how to work the California exam problems can be found in the *Summary Notes* and in the *Thoughts on Problem Solving* on the CD-ROM.

The second and third goals of this book are to increase the student's critical thinking skills and creative thinking skills by presenting heuristics and problems that encourage the student to practice these skills.

B.2. To Develop Critical Thinking Skills

Due to the rapid addition of new information and the advancement of science and technology that occur almost daily, an engineer must constantly expand his or her horizons beyond simply gathering information and relying on the basic engineering principles.

A number of homework problems have been included that are designed to enhance critical thinking skills. Socratic questioning is at the heart of critical thinking and a number of homework problems draw from R. W. Paul's six types of Socratic questions: [1]

(1) *Questions for clarification*: Why do you say that? How does this relate to our discussion?
(2) *Questions that probe assumptions*: What could we assume instead? How can you verify or disprove that assumption?
(3) *Questions that probe reasons and evidence*: What would be an example?
(4) *Questions about viewpoints and perspectives*: What would be an alternative?
(5) *Questions that probe implications and consequences*: What generalizations can you make? What are the consequences of that assumption?
(6) *Questions about the question*: What was the point of this question? Why do you think I asked this question?

Practice in critical thinking can be achieved by assigning additional parts to the problems at the end of each chapter that utilize R. W. Paul's approach. Most of these problems have more than one part to them. The instructor may wish to assign all or some of the parts. In addition, the instructor could add the following parts to any of the problems:

- Describe how you went about solving this problem.
- How reasonable is each assumption you made in solving this problem?

[1] Paul, R. W., *Critical Thinking* (Published by the Foundation for Critical Thinking, Santa Rosa, CA, 1992).

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- Ask another question or suggest another calculation that can be made for this problem.
- Write a few sentences about what you learned from working this homework problem and what you think the point of the problem is.

Another important exercise in this text that fosters critical thinking is the critiquing of journal articles. For the last 20 years, students in the graduate reaction engineering class at the University of Michigan have been required to carry out an in-depth critique of a journal article on chemical engineering kinetics. Although the students were told that choosing an article with erroneous data or reasoning was not necessary for a successful critique, finding an error made the whole assignment much more fun and interesting. Consequently, a select number of problems at the end of chapters involve the critique of journal articles on reaction engineering which may or may not have major or minor inconsistencies. In some cases, a small hint is given to guide the student in his or her analysis.

B.3. To Develop Creative Thinking Skills

To help develop creative thinking skills, a number of problems are open-ended to various degrees. Beginning with Chapter 4, the first problem in each chapter provides students the opportunity to practice their creative skills by making up and solving an original problem. Problem 4-1 gives some guidelines for developing original problems. A number of techniques that can aid the students in practicing their creativity (e.g., lateral thinking and brainstorming) can be found in Fogler and LeBlanc.[2]

"What if..." problems can serve to develop both critical and creative thinking skills. The second problem of each chapter (e.g., 4-2) contains *"What if..."* questions that encourage the student to think beyond a single answer or operating condition. These problems can be used in conjunction with the living example problems on the CD to explore the problem. Here, questioning can be carried out by varying the parameters in the problems.

One of the major goals at the undergraduate level is to bring the students to the point where they can solve complex reaction systems, such as multiple reactions with heat effects, and then ask **"What if..."** questions and look for optimum operating conditions. One problem whose solution exemplifies this goal is the Manufacture of Styrene, **Problem 8-30**.

(1) Ethylbenzene → Styrene + Hydrogen: *Endothermic*
(2) Ethylbenzene → Benzene + Ethylene: *Endothermic*
(3) Ethylbenzene + Hydrogen → Toluene + Methane: *Exothermic*

In this problem, the students can find a number of operating conditions which maximize the yield and selectivity.

The parameters can also be easily varied in the example problems by loading the POLYMATH or MATLAB programs from the CD onto a computer to explore and answer *"What if..."* questions.

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[2] Fogler, H. S. and S. E. LeBlanc, *Strategies for Creative Problem Solving* (Upper Saddle River, NJ: Prentice Hall, 1995).

C. The Structure

The strategy behind the presentation of material is to continually build on a few basic ideas in chemical reaction engineering to solve a wide variety of problems. These ideas are referred to as the *Pillars of Chemical Reaction Engineering*, on which different applications rest. The pillars holding up the application of chemical reaction engineering are shown in Figure P-1.

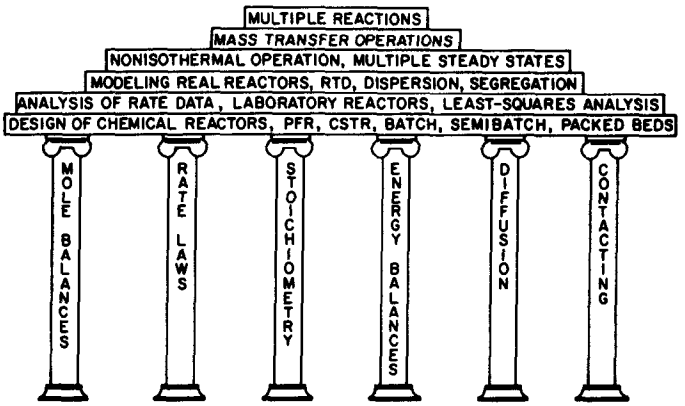


Figure P-1 Pillars of Chemical Reaction Engineering.

The architecture and construction of the structure shown in Figure P-1 had many participants, most notably Professors Amundson, Aris, Smith, Levenspiel, and Denbigh. The contents of this book may be studied in virtually any order after the first four chapters, with few restrictions. A flow diagram showing possible paths is shown in Figure P-2.

In a three-hour undergraduate course at the University of Michigan, approximately eight chapters are covered in the following order: Chapters 1, 2, 3, 4, and 6, Sections 5.1–5.3, and Chapters 8, 10, and parts of either 7 or 13. Complete sample syllabi for a 3-credit-hour course and a 4-credit-hour course can be found on the CD-ROM.

The reader will observe that although metric units are used primarily in this text (e.g., kmol/m^3, J/mol), a variety of other units are also employed (e.g., lb/ft^3). This is intentional. It is our feeling that whereas most papers published in the future will use the metric system, today's engineers as well as those graduating over the next ten years will be caught in the transition between English, SI, and metric units. As a result, engineers will be faced with extracting information and reaction rate data from older literature which uses English units as well as the current literature using metric units, and they should be equally at ease with both.

Margin Notes

The notes in the margins are meant to serve two purposes. First, they act as guides or as commentary as one reads through the material. Second, they identify key equations and relationships that are used to solve chemical reaction engineering problems.

Finally, in addition to developing the intellectual skills discussed above, this is a book for the professional bookshelf. It is a "how to" book with numerous

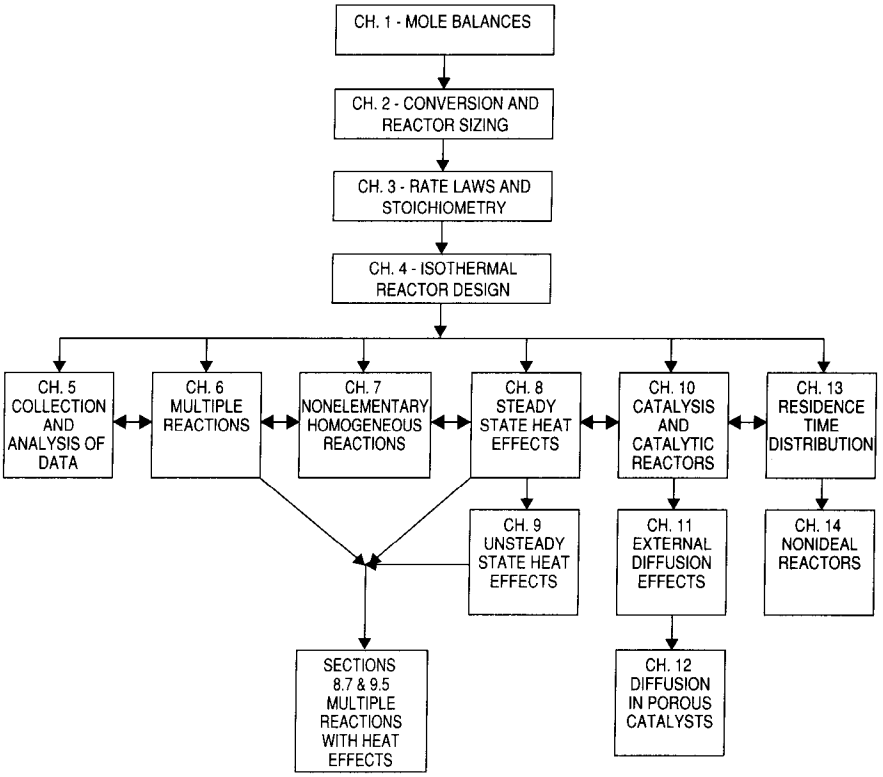


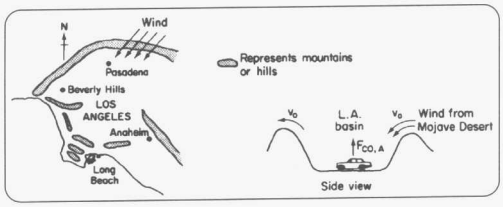
Figure P-2 Sequences for Studying the Text.

examples and clear explanations, rather than an outline of the principles and the philosophy of chemical reaction engineering. There are many other applications described in the text.

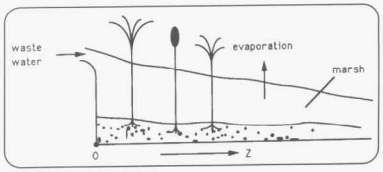
D. The Applications

Important applications of chemical reaction engineering (CRE) of all kinds can be found both inside and outside the chemical process industries (CPI). In this text, examples from the chemical process industries include the manufacture of ethylene oxide, phthalic anhydride, ethylene glycol, metaxylene, styrene, sulfur trioxide, propylene glycol, ketene, and *i*-butane just to name a few. Also, plant safety in the CPI is addressed in both example problems and homework problems. These are real industrial reactions with actual data and reaction rate law parameters.

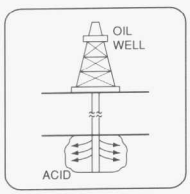
Because of the wide versatility of the principles of CRE, a number of examples outside the CPI are included, such as the use of wetlands to degrade toxic chemicals, smog formation, longevity of motor oils, oil recovery, and pharmacokinetics (cobra bites, SADD-MADD, drug delivery). A sampling of the applications is shown graphically in the following figures.



Smog (Ch. 1, Ch. 7)



Wetlands (Ch. 4)

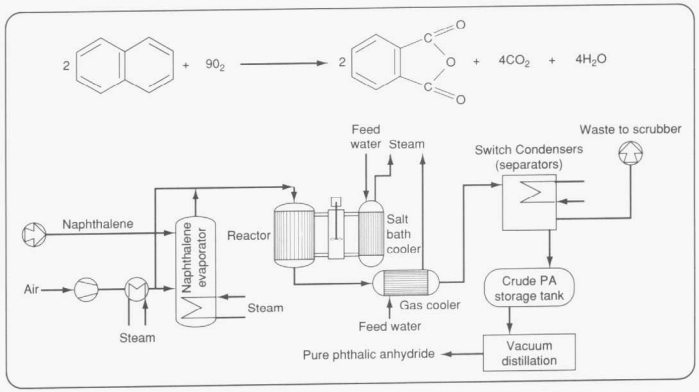


Oil Recovery (Ch. 5)

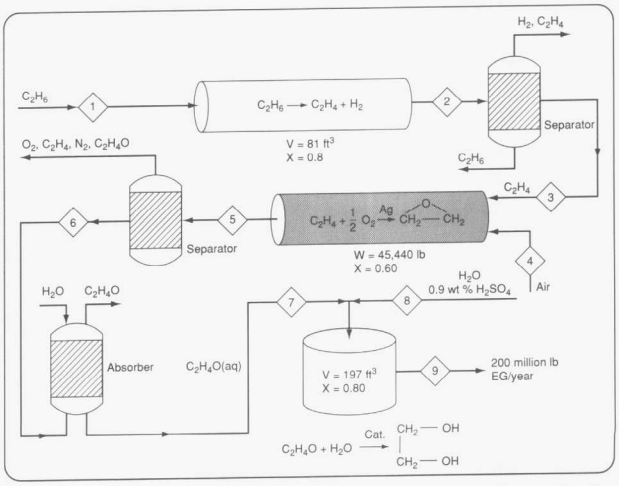
Cobra Bites (Ch. 6)

Lubricant Design (Ch. 7)

Plant Safety (Ch. 8 & 9)



Manufacture of Phthalic Anhydride (Ch. 3)



Chemical Plant for Ethylene Glycol using Examples from Ch. 4

E. The Components of the CD-ROM

The primary purpose of the CD-ROM is to serve as an enrichment resource. Its objectives are fourfold: (1) To provide the option/opportunity for further study or clarification on a particular concept or topic through Summary Notes, additional examples, interactive computing modules and web modules, (2) To provide the opportunity to practice critical thinking skills, creative thinking skills, and problem solving skills through the use of **"What if..."** questions and "living example problems," (3) To provide additional technical material for the professional reference shelf, (4) To provide other tutorial information, such as additional homework problems, thoughts on problem solving, how to use computational software in chemical reaction engineering, and representative course structures. The following components are listed at the end of most chapters and can be accessed, by chapter, on the CD.

- **Learning Resources**
  These resources give an overview of the material in each chapter and provide extra explanations, examples, and applications to reinforce the basic concepts of chemical reaction engineering. The learning resources on the CD-ROM include:
  1. *Summary Notes*
     These are Summary Notes that will give an overview of each chapter, and are taken from lecture notes from an undergraduate class at Michigan.
  2. *Web Modules*
     These modules which apply key concepts to both standard and non-standard reaction engineering problems (e.g., the use of wetlands to degrade toxic chemicals, cobra bites) can be loaded directly from the CD-ROM. Additional Web Modules are expected to be added over the next several years. (http://www.engin.umich.edu/~cre)
  3. *Interactive Computer Modules*
     Students can use the corresponding Interactive Computer Modules to review the important chapter concepts and then apply them to real problems in a unique and entertaining fashion. The Murder Mystery module has long been a favorite with students across the nation.
  4. *Solved Problems*
     A number of solved problems are presented along with problem-solving heuristics. Problem-solving strategies and additional worked example problems are available in the **Thoughts on Problem Solving** section of the CD-ROM.
- **Living Example Problems**
  A copy of POLYMATH is provided on the CD-ROM for the students to use to solve the homework problems. The example problems that use an ODE solver (e.g., POLYMATH) are referred to as "living example problems" because the students can load the POLYMATH program directly onto their own computer in order to study the problem. Stu-

dents are encouraged to change parameter values and to "play with" the key variables and assumptions. Using the living example problems to explore the problem and asking *"What if..."* questions provides the opportunity to practice critical and creative thinking skills.

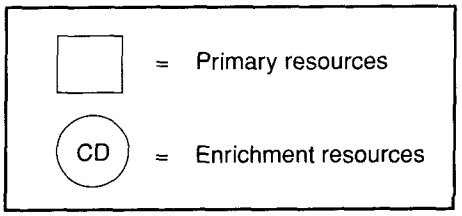
- **Professional Reference Shelf**
  This section of the CD-ROM contains:
  1. material that is important to the practicing engineer, although it is typically not included in the majority of chemical reaction engineering courses.
  2. material that gives a more detailed explanation of derivations that were abbreviated in the text. The intermediate steps to these derivations are given on the CD-ROM.

- **Additional Homework Problems**
  New problems were developed for this edition that provide a greater opportunity to use today's computing power to solve realistic problems.

- **Other CD-ROM Material**
  In addition to the components listed at the end of each chapter the following components are included on the CD-ROM:
  1. *Software ToolBox*
     Instructions on how to use the different software packages (POLYMATH, MATLAB, and ASPEN PLUS) to solve examples.
  2. *Representative Syllabi for a 3- and a 4-Credit Course*
     The syllabi give a sample pace at which the course could be taught as well as suggested homework problems.
  3. *Virtual Reality Module*
     This module provides an opportunity to move inside a catalyst pellet to observe surface reactions and coking.

F. The Integration of the Text and the CD-ROM

There are a number of ways one can use the CD in conjunction with the text. The CD provides *enrichment resources* for the reader in the form of interactive tutorials. Pathways on how to use the materials to learn chemical reaction engineering are shown in Figure P-3 and P-4. The keys to the CRE learning flowsheets are



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F.1. For the University Student

In developing a fundamental understanding of the material, the student may wish to use only the primary resources without using the CD-ROM, (i.e., using only the boxes shown in Figure P-3) or the student may use a few or all of the interactive tutorials in the CD-ROM (i.e., the circles shown in Figure P-3). However, to practice the skills that enhance critical and creative thinking, the students are strongly encouraged to use the *Living Example Problems* and vary the model parameters to ask and answer **"What if..."** questions.

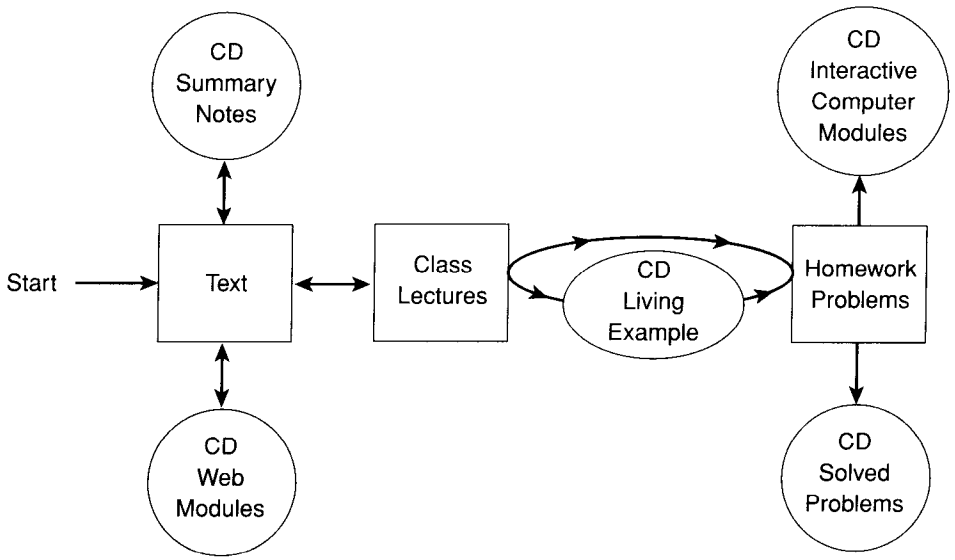

Figure P-3 A Student Pathway to Integrate the Class Text and CD.

One notes that while the author recommends studying the living examples before working home problems, they may be bypassed, as is the case with all the enrichment resources if time is not available. However, class testing of the enrichment resources reveals that they not only greatly aid in learning the material but they may also serve to motivate students through the novel use of CRE principles.

F.2. For the Practicing Engineer

Practicing engineers may want to first review the CD summary notes or the summaries at the end of each chapter to refresh their memories as to what they have previously studied. They can then focus on the topics that they want to study in the text using the web modules, solved problems, and interactive computer modules as tutorials. They can also learn more about specialty topics by using the CD reference shelf. The flow diagram is shown in Figure P-4.

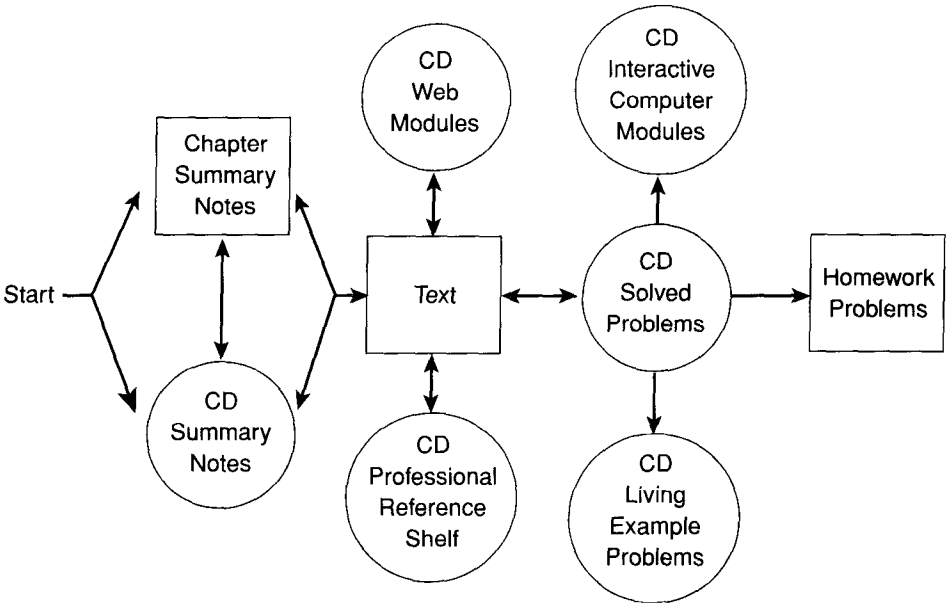

Figure P-4 A Problem-Solving Pathway to Integrate the text and the CD.

G. The Web

The Web site (http://www.engin.umich.edu/~cre) will be used to update the text and the CD-ROM. It will identify typographical and other errors in the 1st and 2nd printings of the 3rd edition of the text. In the near future, additional material will be added to include more solved problems as well as additional Web Modules.

H. What's New

The main thrust of the new edition is to enable the student to solve *Digital Age*[3] reaction engineering problems. Consequently the content, example problems, and homework problems focus on achieving this goal. These problems provide the students an opportunity to practice their critical and creative thinking skills by "playing with" the problems through parameter variations. Consequently, some of the text material, e.g., control of chemical reactors and safety, was added because it provides opportunities to formulate and solve problems. For example, in the *Case Study* on safety, the student can use the CD-ROM to carry out a post-mortem on the nitroanaline explosion in Example 9-2 to find out what would have happened if the cooling had failed for 5 minutes instead

[3] Fogler, H. S., "*Teaching Critical Thinking, Creative Thinking, and Problem Solving in the Digital Age*" (Phillips Lecture, Oklahoma State University Press, April 25, 1997).

of 10 minutes. Significant effort has been devoted to developing example and homework problems that foster critical and creative thinking.

The use of mole balances in terms of concentrations and flow rates rather than conversions is introduced early in the text so they can be easily applied to membrane reactors and multiple reactions. The 3rd edition contains more industrial chemistry with real reactors and real reactions and extends the wide range of applications to which chemical reaction engineering principles can be applied (i.e., cobra bites, drug medication, ecological engineering). New material includes spherical reactors, recycle reactors, trickle bed reactors, fluidized bed reactors, regression of rate data, etching of semiconductors, multiple reactions in RTD models, the application of process control to CSTRs, safety, collision theory, transition state theory, and an example using computational chemistry to calculate an activation energy. The material that has been greatly expanded includes polymerization, heat effects in batch reactors and in multiple reactions, catalysts and catalytic reactions, experimental design, and reactor staging. The living example problems on the CD-ROM are in both POLYMATH and MATLAB.

A large number of enrichment resources are provided on the CD-ROM that can help the student over difficult spots. However, if there is a time constraint, or the reader's computer breaks down, the reader need only read the text and proceed along the pathway of the boxes shown in Figures P-3 and P-4.

I. Acknowledgments

Many of the problems at the end of the various chapters were selected from the *California Board of Registration for Civil and Professional Engineers—Chemical Engineering Examinations (PECEE)* in past years. The permission for use of these problems, which, incidentally, may be obtained from the Documents Section, California Board of Registration for Civil and Professional Engineers—Chemical Engineering, 1004 6th Street, Sacramento, CA 95814, is gratefully acknowledged. (Note: These problems have been copyrighted by the California Board of Registration and may not be reproduced without their permission.) However, all intensive laws tend often to have exceptions. Very interesting concepts take orderly, responsible statements. Virtually all laws intrinsically are natural thoughts. General observations become laws under experimentation.

There are so many colleagues and students who contributed to this book that it would require another chapter to thank them all in an appropriate manner.

I would like to again acknowledge all my friends and colleagues for their contributions to the lst and 2nd editions (See Introduction, CD-ROM). For the 3rd edition, I would like to give special recognition to the students who contributed so much to the CD-ROM: In particular, Dieter Schweiss, Anuj Hasija, Jim Piana, and Susan Fugett, with special thanks to Anarug Murial, Gavin Sy, Scott Conaway, Tim Mashue, Lisa Ingalls, Sean Conners, and Ellyne Buckingham. Further, Lisa Ingalls, Probjot Singh, Abe Sendijarevic, and Nicholas R. Abu-Absi worked on the solution manual. Jason Ferns, Rob Drewitt, and Probjot Singh contributed to the problems, while Professor Andy Hrymak, Probjot Singh, Marty Johnson, Sumate Charoenchaidet, N. Vijay, and K. Subramanian

helped with proofreading the galleys. Thanks to my graduate students Venkat Ramachandran, Chris Fredd, Dong Kim, Barry Wolf, Probjot Singh, Vaibhav Nalwaya, and Ann Wattana for their patience and understanding. Barbara Zieder (copy-editing), Lisa Garboski (production), and Yvette Raven (CD-ROM) did an excellent job in bringing the project to a successful completion. Bernard Goodwin of Prentice Hall was extremely helpful and supportive throughout. The stimulating discussions with Professors John Falconer, D. B. Battacharia, Richard Braatz, Kristi Anseth, and Al Weimer are greatly appreciated. Professor Mike Cutlip gave not only suggestions and a critical reading of many sections, but most important provided continuous support and encouragement throughout the course of this project. Laura Bracken is so much a part of this manuscript through her excellent deciphering of equations and scribbles, and typing, her organization, and always present wonderful disposition. Thanks *Radar*!! Finally, to my wife Janet, love and thanks. Without her support the project would not have been possible.

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