Elements of Chemical Reaction Engineering

Second Edition

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H. SCOTT FOGLER

Ame and Catherine Vennema Professor
of Chemical Engineering
The University of Michigan, Ann Arbor

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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

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 from those at the end of each chapter. Most problems requiring significant numerical computations can be solved with a personal computer which has at least BASIC as a programming language.

The thrust of this book is to present in a clear and concise manner the fundamentals of chemical reaction engineering. First, a structure is developed 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. In perhaps no other area of engineering is mere formula plugging more hazardous; the number of physical situations in reaction engineering that can arise appears infinite, and the chances of a simple formula being sufficient for the adequate design of a real reactor are vanishingly small. However, the algorithms presented in the text for reactor design provide a framework with which one can develop confidence through reasoning rather than memorization.

Due to the rapid addition of new information and scientific principles, a true engineer must constantly expand his or her horizons beyond simple gathering of information and engineering principles. Thus the second goal of this book is to increase the student's lifelong learning skills by presenting heuristics and problems that encourage the student to practice certain intellectual skills. 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.

Another important skill fostered in this text is a critical analysis of journal articles. For the last ten years students in the graduate reactor 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, it was stated that finding an error made the whole assignment much more fun. Consequently, a select number of problems at the end of chapters involve the critique of journal articles on reactor 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.

Many of the problems at the end of the various chapters were selected from those which have appeared in California Board of Registration for Civil and Professional Engineers—Chemical Engineering Examinations (PECEE) over 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 many not be reproduced without their permission.) Additional problems are available on diskettes for use with the personal computer. Information about these interactive programs may be obtained from the author.

The strategy behind the presentation of material is the application, modification, or extrapolation of several 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.

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, Sections 5.1–5.3, 6.1–6.5, and Chapters 8, 10, 11, and parts of 13.

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

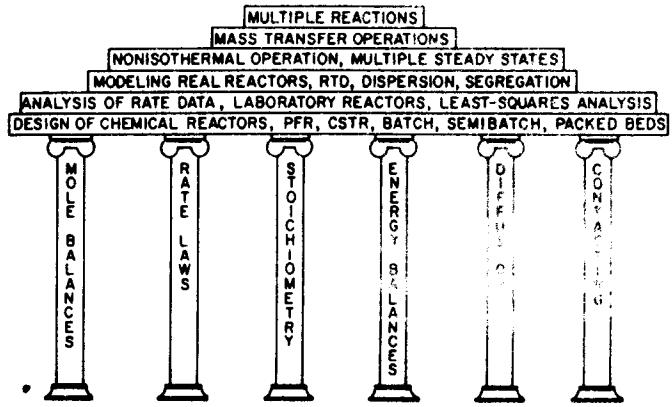

Figure P-1 Pillars of Chemical Reaction Engineering

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, and should be equally at ease with both.

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

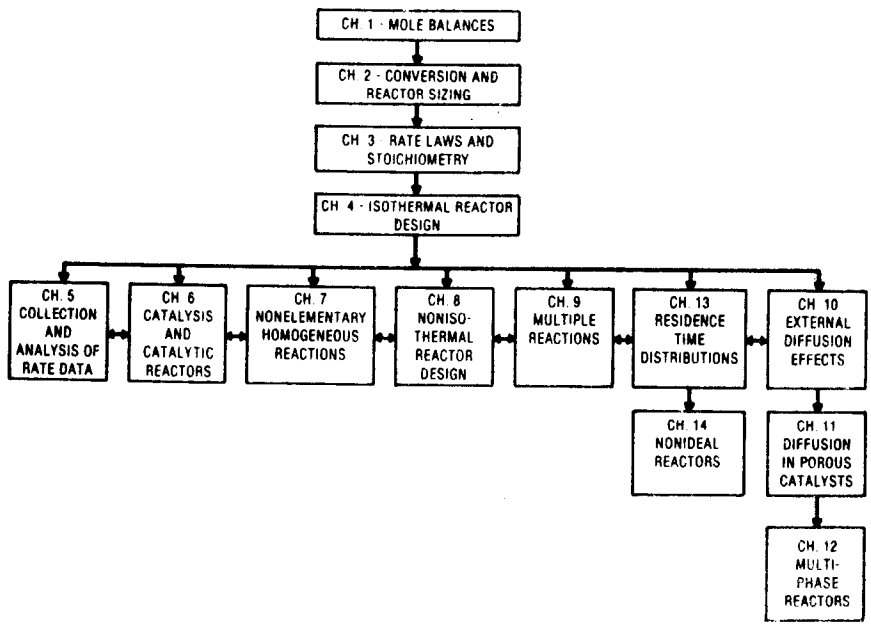

Figure P-2 Sequences for Studying the Text

I had not anticipated undertaking a revision of the text after only six years, but a number of major changes have taken place in our profession since the original manuscript was submitted for publication in 1984. First of all, there has been a paradigm shift in the solution to reaction engineering problems as a result of the fantastically user-friendly O.D.E. (Ordinary Differential Equation) Solvers. This shift is similar to the shift that came about when we went from slide rules to hand-held calculators in the mid 1970's.

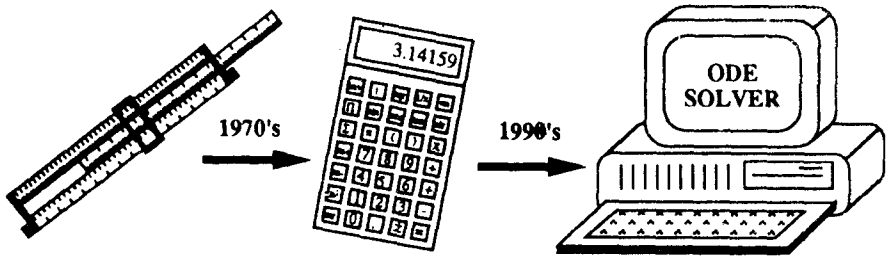

Figure P-3 Paradigm Shifts in Chemical Engineering Education

In addition to the advances in computer hardware and software, there also has been an increase in the computer literacy of our students. Consequently, there is an increased emphasis in the second edition on numerical solutions to reaction engineering problems. Students are expected to either write their own programs to solve ordinary differential equations (O.D.E.) and non-linear algebraic equations, or to use software packages (O.D.E. Solvers) currently available for this purpose such as **POLYMATH** and **MATHEMATICA**. With the O.D.E. and non-linear algebraic software packages, a greater emphasis can be placed on having students explore the solutions through a parameter sensitivity analysis. They can carry out small investigations on the effect of various parameters or variable settings and then write a paragraph describing their findings. Many of the solutions to the example problems use both an O.D.E. Solver and a computer program; however, the use of a software package, such as **POLYMATH**, has recently become the author's strong preference for solving reaction engineering problems.

POLYMATH has been offered by the CACHE Corporation to all Chemical Engineering Departments in the United States and Canada for unlimited use by faculty and students. It can also be individually purchased directly from the CACHE Corporation for a *very* nominal charge.

CACHE Corporation P.O. Box 7939 Austin, Texas 78713-7379	Mathematica for Macintosh % Wolfram Research 100 Trade Center Drive Champaign, Illinois 61820-9910	Maple Waterloo Maple Software 766884 Ontario, Inc. 160 Columbia St. West Waterloo, Ontario Canada N2L3L3

POLYMATH and Maple can be used with an IBM-compatible P.C.; for Macintosh users, Mathematica and Maple are available.

In addition to the changes in computer technology, a number of emerging technologies, namely, microelectronics processing and biotechnology, have recently found their way into the mainstream of chemical engineering. Material in these areas has been included in the second edition and follows directly from the basic principles of chemical reaction engineering. In addition to these areas, more traditional topics have been added, such as the shrinking core model, the approach to the steady state (temperature-concentration phase-planes), polymerization, along with a complete revision of the analysis of multiple reactions. Hopefully, all intensive laws tend often to have exceptions. Very interesting concepts take orderly, responsible statements. Virtually all laws instinctively are normal thoughts. General observations become laws under experimentation.

Acknowledgements

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. Unfortunately, since Prentice-Hall has already requested a page limitation, this is not possible. However, certain people should not go unacknowledged.

In addition to collaborating on Chapters 13 and 14, Dr. Lee Brown provided material for Chapters 3, 6, and 8, and gave a critical reading of the first edition of the text. Lee's insights and friendship contributed greatly to this project. The first edition of this book would never have been completed were it not for Susan Montgomery, an alumna of my undergraduate chemical reaction course. Susan typed, retyped, edited, pasted, proofread, and commented on the entire book many times in addition to handling the many details associated with putting the manuscript in final form.

I would like to thank several of my colleagues for their help: Professor Mike Cutlip of the University of Connecticut, for educating me on the use of O.D.E. Solvers in reaction engineering problems; Professors John Falconer of the University of Colorado; Cam Crowe of McMaster University, and again Mike Cutlip, for showing me that the best way to analyze complex *multiple reaction problems* is to use molar flow rates and concentrations rather than conversion.

I also appreciate the many stimulating discussions I have had with Professors Rane Curl and Phillip Savage of our department. These discussions helped clarify my thinking and led me to new ways of presenting some of the new material, as well as ways of revising some sections of the old edition.

Also, I acknowledge Laura Bracken and Mary Reeves, who were superb, not only for their excellent typing, but for their patience in preparing an endless number of drafts of revised material. John Gyenese, the depart-

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HSF
Ann Arbor

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