PREFACE

Book Overview

This book provides extensive problem-solving instruction and suggestions, numerous examples, and many complete and partial solutions in the main subject areas of chemical and biochemical engineering and related disciplines. Problem solutions are clearly developed using fundamental principles to create mathematical models. An equation-oriented approach that enables computer-based problem solving on personal computers is utilized. Efficient and effective problem solving is introduced employing numerical methods for linear equations, nonlinear equations, ordinary and partial differential equations, linear and nonlinear regressions, and polynomial curve fitting. Basic to advanced problem solving is covered utilizing a novel integrated approach with three widely used mathematical software packages: POLYMATH, Excel, and MATLAB. Readers may choose to focus on one or more of these software packages or utilize another mathematical software package.

The book and a dedicated web site (**www.problemsolvingbook.com**) furnish all necessary problem information, software files, and additional enrichment materials. For advanced applications, unique software tools are provided for solving complex problems such as parameter estimation in dynamic systems and solution of constrained systems of algebraic equations.

Intended Audience

This book is intended for individuals who are interested in solving problems in chemical and biochemical engineering and in related fields by using mathematical software packages on personal computers. It can serve as a textbook for students in conjunction with college- and university-level courses, and it can be a companion reference book for individual students. For professionals, it can be an invaluable reference book that also allows extensive self-study in problem solving using the most widely used software packages.

Background

Prior to the introduction of the personal computers and mathematical software packages in the early 1980's, desktop calculations for engineering problem solving were mainly carried out with hand-held calculators. Sometimes mainframe computers were utilized, which required source code programming. Since then the emphasis has gradually moved to computer-based (or computer-enhanced) problem solving or CBPS on desktop or notebook computers. By the time the first edition of this book was published in 1999, it became evident that CBPS can be a

very important, or possibly the most important, application of the computer in scientific and engineering education and in industrial practice.

The first edition of this book provided examples to the use of CBPS in core chemical engineering subject areas using the POLYMATH software package. Shortly after the publication of the first edition, we carried out several comparison studies in order to determine what types of software packages should be included in the "toolbox" of the engineering student and the practicing engineer that would enable the effective and efficient solution of practical problems. We arrived at the conclusion that three types of software are needed. There is a need for a numerical problem solver, such as POLYMATH, that accepts the model equations close to their mathematical forms and provides their numerical solution with very minimal user intervention. Additionally, there is also a need to be able to use spreadsheet software, such as Excel, because of its wide use in business and industry. Software like Excel is also used for the organization and presentation of information in tabular and graphical forms and for database management-related operations. Software packages that support programming, such as MATLAB, are needed to implement algorithms which are required in graduate research and advanced mathematics, programming, control, and numerical analysis courses.

It is increasingly important for today's engineering student and forward-looking engineering professionals to be proficient in the use of several software packages, and thus we greatly expanded the book so that it now includes solutions in Excel and MATLAB, in addition to POLYMATH. New problems have been introduced that demonstrate how the special capabilities of each of these packages can best be utilized for efficient and effective problem solving.

The POLYMATH Numerical Computation Package

The POLYMATH package provides convenient solutions to most numerical analysis problems, including the problems that are presented in this book. We authored and published the first PC version of POLYMATH in 1984, and it has been in use since then in over one hundred universities and selected industrial sites world wide. The version available at the time of the publication of the book, POLYMATH 6.1, was released in 2006. This package contains the following programs:

- Ordinary Differential Equations Solver
- Nonlinear Algebraic Equations Solver
- Linear Algebraic Equations Solver
- Polynomial, Multiple Linear, and Nonlinear Regression Program

The programs are extremely easy to use, and all options are menu driven. Equations are entered in standard form with user-defined notation. Results are presented in graphical or tabular form. A sophisticated calculator and a general unit conversion utility are available within POLYMATH.

The new and unique capability of the latest POLYMATH to automatically export any problem to Excel and MATLAB with a single keypress is extensively

utilized within this book. Automatic export to Excel includes all intrinsic functions and logical variables. A POLYMATH ODE_Solver Add-In is included for solving ordinary differential equations in Excel. Upon export to MATLAB, the equations are ordered in the computational sequence, the intrinsic functions and logical statements are converted, and a MATLAB function is generated. Template files to run the functions are available in the HELP section of POLYMATH or from the book web site.

Current information on the latest POLYMATH software is available from

www.polymath-software.com

Many departments and some universities have obtained site licenses for POLYMATH. These licenses allow installation in all computer labs, and individual copies can be provided to all students, faculty and staff for use on personal computers. Detailed information is available from

academic@polymath-software.com

Use of This Book

This book is intended to serve as a companion text for the engineering student, the faculty instructor, or the practicing engineer. The instructions in the practical use of mathematical software package on representative problems from most chemical and biochemical engineering subject areas provide direct insight into problem setup and various practical aspects of numerical problem solving.

For the undergraduate student at the early stages of his/her studies, the book can serve as the textbook for learning to categorize the problems according to the numerical methods that should be used for efficient and effective solutions. It provides basic instruction in the use of three popular and widely used software packages: POLYMATH, Excel, and MATLAB. Emphasis is on setting up problems and effectively obtaining the necessary solutions.

In addition to providing general numerical solving capabilities, the text gives problems in most subject areas so that it can serve as a reference book in most courses, as it provides example problems that can be illustrative of problems that may be assigned in the various courses. The book also provides help with problem solving in advanced level for problems often encountered in undergraduate and graduate research such as nonlinear regression, parameter estimation in differential systems, solving two-point boundary value problems and partial differential equations, constrained equation solving, and optimization.

For the practicing engineer, the book serves as resource book in computer-based problem solving. It provides a solid foundation in problem solving and can develop basic and advanced skills in the utilization of spreadsheets. Practical problems illustrate various problem solving approaches that can be implemented for problem formulation, problem solving, analysis, presentation of results, and documentation. Of particular interest is the coverage of the correlation and regression of data with statistical analysis. All of the book's problems can be solved with the Excel spreadsheet software that is widely used in industry.

Engineering faculty can use the book to introduce numerical methods into an individual course, a sequence of courses, or an entire departmental curriculum. This book provides supplementary problems that can be assigned to students in order to introduce numerical problem solving which is avoided in most textbooks. Many of the problems can be easily extended to open-ended problem solving so that critical thinking skills can be developed. The numerical solutions can be used to answer many "what if" type questions so that students can be encouraged to think about the implications of the problem solutions. The book can also be used as a companion textbook for an introductory computer programming course or a comprehensive course in numerical analysis.

Book Organization

All the chapters of the book, except the introductory Chapter 1, are built around problems that serve to provide practical applications in a particular subject area. Most of the problems presented in the book have the same general format for the convenience of the reader. The concise problem topic is followed by a listing of the engineering concepts demonstrated by the problem. Then the numerical methods utilized in the solution are indicated just before the detailed problem statement. Each of the problems presents the detailed equations and parameter values that are necessary for solution, including the appropriate units in a variety of systems, with Systéme International d'Unités (SI) being the most commonly used. Because of the wide variety of problems posed in this book, the notation used has been standardized according to one of the major Prentice Hall textbooks in the various subject areas whenever possible. Physical properties are either given directly in the problem or in the appendices.

The book is divided into two parts. In the first part, which includes the first six chapters, subjects of general interest are presented, some on an introductory level and some on an advanced level. In Chapter 1, Introduction, the history of CBPS is briefly reviewed and guidelines are provided for categorizing problems according to the numerical techniques that should be used for their solution. Chapter 2, Basic Principles and Calculations, serves a dual purpose. The chapter introduces the reader to the subject material that is typically taught in a first chemical engineering course (in most universities called Material and Energy Balance, or Stoichiometry). Additionally, this chapter demonstrates the use of POLYMATH for solving simple problems belonging to the main categories discussed in the book, namely single nonlinear algebraic equations, systems of linear algebraic equations, linear and polynomial regression, and systems of ordinary differential equations (ODEs). In Chapter 3, Regression and Correlation of Data, the application of POLYMATH for analysis and regression of data using advanced statistical techniques is demonstrated. Chapter 4, Problem Solving with Excel, introduces the reader to the engineering and scientific problem solving capabilities of Excel using problems belonging to the same categories as in Chapter 2. The automatic export capabilities of POLYMATH to Excel are discussed. More advanced topics such as solution of systems of nonlinear algebraic equations (NLEs) and optimization with constraints (nonlinear programming) are also presented. In Chapter 5, Problem Solving with MATLAB, MATLAB is

used to solve the problems presented in Chapter 4. The capability of POLYMATH to automatically generate MATLAB m-files are presented and provided templates for MATLAB problem solutions are demonstrated and utilized. In Chapter 6, Advanced Techniques in Problem Solving, the problem solutions deal with advanced topics such as two-point boundary value problems, systems of differential-algebraic equations, partial differential equations, and parameter estimation in systems of differential equations.

The second part of the book (Chapters 7 through 14) is organized according to the particular subject areas such as Thermodynamics (Chapter 7), Fluid Mechanics (Chapter 8), and so forth. The content of these chapters is presented in the typical order of coverage in college or university-level courses.

New Content in the Second Edition

The contents of the book were almost doubled by adding six new chapters to the eight chapters of the first edition. The introductory Chapter 1 was added in order to help the reader in a very critical step of the problem solving—the characterization of the problem in terms of the solution method that has to be used.

After studying and verifying the importance of various software packages in effective and efficient problem solving, the two chapters dealing with the use of Excel and MATLAB were added. These chapters also introduce the new capability of the POLYMATH software to automatically convert a problem solution into Excel worksheets and MATLAB m-files. This considerably shortens the learning curve associated with the initial use of these packages.

Since the first edition was published, biochemical engineering has gained importance and is now being taught in most colleges and universities. The new biochemical engineering chapter and selected problems in other chapters provide a wide selection of problems in this important subject area. New chapters on "Phase Equilibria and Distillation" (Chapter 12) and "Process Dynamics and Control" (Chapter 13) have been added.

Companion Web Site

Readers of the book are encouraged to make full use of the companion web site that will be maintained and extended by the book's authors. This web site enable downloads of programs files which are used in the various book chapters for the three software packages: POLYMATH, Excel, and MATLAB. Additional educational problems, learning resources, corrections and updates to this book, and new materials are provided.

www.problemsolvingbook.com/

The web site also allows book owners to purchase and immediately download the latest POLYMATH software at significant discounts from the already highly discounted POLYMATH Educational version software. This enables book users to have the very latest software at very reasonable cost.

Instructors who are using the book have special access to all problems as well as substantial educational and enrichment materials through the companion web site. This include suggestions as to the book use in individual courses, sequences of courses, and throughout a departmental curriculum. Details about this access are provided in Chapter 1 from the authors.

Recommendation for Book Use in Various Courses

There are many ways this book can be utilized in a variety of engineering and related courses. Some of the problem suggestions for courses are listed here.

1. Basic Principles and Calculations (or Material and Energy Balance or Stoichiometry): All of Chapter 2, Problems 4.1 and 5.1.
2. Thermodynamics: Problems 2.1 and 2.2, 2.5 through 2.13, 3.1 through 3.4, 3.8, 3.9, 3.14, 4.1, 4.4, 4.5, 5.1, 5.4, 5.5, 6.6, all of Chapter 7, and Reference No. 9 in Table 1.
3. Fluid Mechanics: All of Chapter 8, Problems 4.2, 5.2, 10.15, and Reference No. 2 in Table 1.
4. Heat Transfer: All of Chapter 9 and Problems 2.16, 3.5, 3.6, 3.7, 6.8, 10.12, 11.22, 11.23, 11.24, 11.25, 13.6 through 13.12, 13.14, and Reference No. 4 in Table 1.
5. Mass Transfer: All of Chapter 10 and Problems 6.5, 11.4, 11.26, 14.5, 14.16, and 14.17.
6. Chemical Reaction Engineering: All of Chapters 11 and 14, Problems 3.10 through 3.13, 4.3, 4.5, 5.3, 5.5, 6.1 through 6.6, 10.5 through 10.7, 10.11, 10.14, 10.15, 13.3, 13.12, 13.14, 13.15, and References No. 1 and 3 in Table 1.
7. Phase Equilibria and Distillation: All of Chapter 12, Problems 2.10, 2.11, 2.12, 3.8, 3.9, 3.14, 6.8, 7.8, through 7.12, and Reference No. 6 in Table 1.
8. Process Dynamics and Control: All of Chapter 13, Problems 2.14, 2.15, 2.16, 6.1, 6.2, 6.3, 6.8, 6.9, 8.14 through 8.17, 9.11 through 9.14, 10.3, 10.4, 10.13, 10.14, 11.5, 11.18, 11.20, 11.21, 11.22, 11.28, 12.10, 12.11, 14.1, 14.4, 14.6 through 14.10, 14.12, 14.13, 14.16, 14.17, and Reference No. 1 in Table 1.
9. Biochemical Engineering: All of Chapter 14 and Problems 2.3, 6.1, 6.9, 11.20, 11.27, 11.28, 12.11, 13.14, and 13.15.
10. Advanced Mathematics, Numerical Methods, and Systems of NLEs: Problems 4.5, 5.5, 6.4, 6.6, 6.7, 7.12, 7.13, 10.2, 13.2, and 13.3. Note that a MATLAB function for solving systems of constrained NLEs is provided.
    - ODEs—Boundary Value Problems: Problems 6.5, 6.6, 8.1 through 8.4, 8.18, 9.2 through 9.7 10.1, 10.3, 10.5 through 10.10, 10.12, and 14.5.
    - Differential Algebraic Equations: Problems 6.8 and 13.10, and Reference No. 6 in Table 1.
    - Stiff Systems of ODEs: Problems 6.2, 6.3 and 6.4.
    - Partial Differential Equations: Problems 6.9, 8.17, 8.18, 9.12, 9.13, 9.14, 10.13, 10.14, and 10.15.
    - Nonlinear Regression: Problems 2.12, 2.13, 4.4, 5.4, 11.7, 14.7, and 14.8.
11. Applied Statistics: All of Chapter 3, Problem 6.10 and References Nos. 3 and 8 in Table 1.
12. Nonlinear Programming: Problems 4.5, 5.5, 6.9, 14.4, 14.6, 14.11 through 14.16.

13. Process Safety: References No. 7, 10, and 12 in Table 1.

14. Environmental Engineering: Reference No. 11 in Table 1.

15. Introduction to Computer Based Problem Solving: This course can compliment or replace the traditional programming course. This book can serve as the primary textbook for such a course. Content can include Chapters 1 and 2, Problems 3.3, 3.4, 3.5, 3.6, 4.1, 4.2, 4.4, 5.1, 5.2, and 5.4. Problems 2.14 and 8.8 can be used to introduce NLEs and ODEs at the introductory level as replacements for Problems 4.3 and 5.3.

Table 1 Additional Problem References

No.	Title and Reference
1	"Exothermic CSTR's—Just How Stable are the Multiple Steady States?" *Chem. Eng. Educ.*, *28*(1), 30-35 (1994).
2	"Numerical Experiments in Fluid Mechanics with a Tank and Draining Pipe," *Comput. Appl. Eng. Educ*, *2*(3), 175-183 (1994).
3	"Correlation and Over-correlation of Heterogeneous Reaction Rate Data," *Chem. Eng. Educ.*, *29*(1) 22-25, 45 (1995).
4	"The Wind-Chill Paradox: Four Problems in Heat Transfer," *Chem. Eng. Educ.*, *30*(4), 256-261 (1996).
5	"Replacing the Graph Paper by Interactive Software in Modeling and Analysis of Experimental Data," *Comput. Appl. Eng. Educ.*,*4*(3), 241-251 (1996).
6	"What To Do If Relative Volatilities Cannot Be Assumed To Be Constant?—Differential-Algebraic Equation Systems in Undergraduate Education," *Chem. Eng. Educ.*, *31*(2), 86-93 (1997).
7	"Prediction and Prevention of Chemical Reaction Hazards—Learning by Simulation," *Chem. Eng. Educ.*, *35*(4), 268-273 (2001).
8	Letter to the Editor Concerning "An Undergraduate Course in Applied Probability and Statistics," *Chem. Eng. Educ.*, *36*(4), 263, 277 (2002).
9	"An Exercise for Practicing Programming in the ChE Curriculum—Calculation of Thermodynamic Properties Using the Redlich-Kwong Equation of State," *Chem. Eng. Educ.*, *27*(2), 148 (2003).
10	Letter to the Editor Concerning "Evaluations of Kinetic Parameters and Critical Runaway Conditions in the Reaction System of Hexamine-Nitric Acid to Produce RDX in a Non-Isothermal Batch Reactor," *Journal of Loss Prevention in the Process Industries*, *17*(6), 513-514 (2004).
11	"Applications of Mathematical Software Packages for Modeling and Simulations in Environmental Engineering Education," *Environment Modeling and Software*, *20*, 1307-1313 (2005).
12	"Combining HAZOP with Dynamic Simulation—Applications for Safety Education," *Journal of Loss Prevention in the Process Industries, 19*, 754 (2006).

Chemical and Biochemical Engineering Departments

Academic departments are encouraged to consider adopting this book during the first introductory course in chemical and/or biochemical engineering and then utilizing the book as a supplement for many of the following courses in the curriculum. This allows an integrated approach to the use of numerical methods throughout the curriculum. This approach can be helpful in satisfying the ABET requirements for appropriate computer use in undergraduate studies.

A first course in numerical methods can also utilize many of the problems as relevant examples. In this application, the book will supplement a standard numerical methods textbook. Students will find the problems in this book to be more interesting than the strictly mathematical or simplified problems presented in many standard numerical analysis textbooks.

Acknowledgments

We would like to express our appreciation to our wives and families who have shared the burden of this effort which took longer than anticipated to complete. We particularly thank Professor H. Scott Fogler for his encouragement with this book effort and with the continuing development of the POLYMATH package. Many thanks are due to Professor Neima Brauner for her help in developing many of the problems.

Additionally, we appreciate the input and many suggestions of our students, who have been subjected to preliminary versions of the problems and have endured the various pre-release versions of the POLYMATH software over the years.

During the twenty-three years that POLYMATH has been in use, many of our colleagues provided advice and gave us help in revising and improving this software package. In particular, we would like to acknowledge the assistance of Professors N. Brauner, B. Carnahan, D. J. Cooper, H. S. Fogler, D. M. Himmelblau, D. S. Kompala, S. E. LeBlanc, E. M. Rosen, and J. D. Seader. H. S. Fogler has also provided some of the problems included in the book.

Continuing development of the POLYMATH program has been a continuing process. The initial programming and algorithm implementations were carried out and maintained for the first ten years by Orit Shacham. She spent many hours and most of her vacations fixing bugs and writing new code for still another version of POLYMATH. She always amazed us by the speed and precision with which she converted ideas into computer code.

For the last seven years, POLYMATH has been coauthored and programmed by Michael Elly. He has developed a very intuitive and user-friendly interface for interactive problem solving. He has also exhibited a unique capability for effectively implementing rather difficult algorithmic challenges. His creativity, organization, speed, and accuracy continue to impress us. We are happy to have him as a continuing member of our team.

The first draft of the first edition this book was typed (and retyped) by Michal Shacham. She took several months of vacation from her job to learn to use various word processors and graphical programs. The draft she typed became the basis for class testing and refinement of the book. Nancy Neborsky

Pickering learned the FrameMaker desktop publishing package and professionally entered the initial materials into the book format for the first edition.

The authoring of this book and the POLYMATH computer software are both very expensive endeavors in both resources and time. We are indebted to our universities, the University of Connecticut and the Ben-Gurion University of the Negev, for the continuous support we have received. The CACHE Corporation (Computer Aids for Chemical Engineering Education) has been very helpful in advancing and promoting the academic use of POLYMATH.

Michael B. Cutlip
Storrs, Connecticut

Mordechai Shacham
Beer-Sheva, Israel