Problem Solving in Chemical Engineering with Numerical Methods

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PREFACE

Intended Audience

This book is for the chemical engineering student or the professional engineer who is interested in solving problems that require numerical methods by using mathematical software packages on personal computers. This book provides many typical problems throughout the core subject areas of chemical engineering. Additionally, the "nuts and bolts" or practical applications of numerical methods are presented in a concise form during example problem solving, which gives detailed solutions to selected problems.

Background

The widespread use of personal computers has led to the development of a variety of tools that can be utilized in the solution of engineering problems. These include mathematical software packages like MathCAD,* Maple,† Mathematica,‡ Matlab,• Polymath,# and spreadsheets like Excel.¶ While there is great potential in the hands of individual PC users, often this potential is not well developed in current engineering problem solving.

In the past the computer was used only for the difficult tasks of rigorous modeling and simulation of unit operations, processes, or control systems, while the routine calculations were carried out using hand-held calculators (or spreadsheet programs more recently), using essentially the same techniques that were used in the slide rule era. Limiting the use of the computer solely to the difficult tasks was justified before the introduction of interactive numerical packages because the use of the computer was very time consuming.

A typical computer assignment in that era would require the student to carry out the following tasks: (1) Derive the model equations for the problem at hand, (2) find an appropriate numerical method to solve the model, (3) write and debug a FORTRAN program to solve the problem using the selected numerical algorithm, and (4) analyze the results for validity and precision.

It was soon recognized that the second and third tasks of the solution were minor contributions to the learning of the subject matter in most chemical engineering courses, but they were actually the most time consuming and frustrating parts of a computer assignment. The computer enables students to solve realistic problems, but the time spent on the technical details that were of minor rele-

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† Maple is a trademark of Waterloo Maple, Inc. (http://maplesoft.com)
‡ Mathematica is a trademark of Wolfram Research, Inc. (http://www.wolfram.com)
• MATLAB is a trademark of The Math Works, Inc. (http://www.mathworks.com)
POLYMATH is copyrighted by M. B. Cutlip and M. Shacham (http://www.polymath-software.com)
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vancy to the subject matter was much too long.

The introduction of interactive numerical software packages brought about a major change in chemical engineering calculations. This change has been called a "paradigm shift" by Fogler.[2] Using those packages the student's (or the practicing engineer's) main task is to set up the model equations. The interactive program provides accurate solutions to these equations in a short time, displaying the results in graphical and numerical forms. The meaning of the paradigm shift, however, is that using the old calculation techniques with the new computer tools brings very little benefit. This is emphasized in the following observation made by deNevers and Seader[1]: "Since the advent of digital computers, textbooks have slowly migrated toward computer solutions of examples and homework problems, but in many cases the nature of the examples and problems has been retained so that they can be solved with or without a computer."

In most of the examples and problems provided in this book, new solution techniques are presented that require the use of the computer. Thus the full benefits of a computer solution can be gained even for routine, simple problems, not just for complicated ones.

In spite of many available numerical problem-solving packages, advanced problem solving via personal computers continues to be under utilized in chemical engineering education. A recent survey by Jones[5] has indicated that "across the country, computers are usually not used effectively in undergraduate engineering science courses. Often they are not used at all. Problem solving approaches and calculation methods are little influenced by the availability of computers." There are several major reasons for this situation.

First, many of the current engineering textbooks and reference books have been very slow to react to the enhanced problem-solving capabilities that are currently available. Unfortunately, the current textbooks in most engineering subject areas have been slow to react to this emerging capability. The lack of properly framed standard problems in various engineering disciplines is accompanied by a lack of faculty interest in the use of new tools and the creation of appropriate problems that utilize these tools.

Another important reason for the lack of mathematical software usage for advanced problem solving is the actual cost of the software for individual students. While there are many educational benefits to having problem solving close at hand on student-owned personal computers, often the cost to the individual students is prohibitively high. Fortunately, the costs to major colleges and universities for site licenses for the use of software only in computer labs is much more reasonable. However, this pricing structure forces students to use problem-solving software only in computer labs and does not allow interactive use of the software at other locations. Thus advanced problem-solving capabilities are not currently as close at hand as the nearest personal computer.

Finally, there is a significant learning curve to most of the advanced problem-solving software. This requires users to become familiar with a command structure that is often not intuitive and thus difficult to use. This is a significant impediment to student, professional, and faculty use of many packages.

Purposes of This Book

The main purpose of this book is to provide a comprehensive selection of chemical engineering problems that require numerical solutions. Many problems are completely or partially solved for the reader. This text is intended to be supplementary to most of the current chemical engineering textbooks, which do not emphasize numerical solutions to example and posed problems. This book is highly indexed, as indicated in Tables 1-9 at the end of this preface. The reader can only consider a particular subject area of interest or the application of a particular numerical method in actual problem solving. In either area, problems or methods, the book gives concise and easy-to-follow treatments.

The problems are presented in a general way so that various numerical problem-solving computer packages can be utilized. Many of the problems are completely solved so as to demonstrate a particular problem-solving approach. In other cases, problem-solving skills of the reader need to be applied.

This book has been designed for use with any mathematical problem solving package. The reader is encouraged to use the mathematical software package of his or her choice to achieve problem solutions. However, the POLYMATH package has been used as an example package, and a complete version of POLYMATH is included in the CD-ROM that accompanies this text. This allows the convenient use of POLYMATH throughout the book, as many of the problems have some part of the solution in POLYMATH files that are available on the CD-ROM.

General Problem Format

All problems presented in the book have the same general format for the convenience of the reader. The concise problem topic is first followed by a listing of the chemical engineering concepts demonstrated by the problem. Then the numerical methods utilized in the solution are indicated just before the detailed problem statement. Typically a particular problem presents all of the detailed equations that are necessary for solution, including the appropriate units in a variety of systems, with Système International d'Unités (SI) being the most commonly used. Physical properties are either given directly in the problem or in the appendices.

Students

Students will find the chapter organization of the book, by chemical engineering subject areas, to be convenient. The problems are organized in the typical manner in which they are covered in most courses. Complete solutions are given to many of the problems that demonstrate the appropriate numerical methods in problem solving. Practice and application of various numerical methods can be accomplished by working through the problems as listed in Table 9.

Practicing Engineers

Engineers in the workplace face ever-increasing productivity demands. Thus the concise framework of the problems in this book should aid in the proper formulation of a problem solution using numerical methods.

Faculty

This book can assist faculty members in introducing numerical methods into their courses. This book is intended to provide supplementary problems that can be assigned to students. 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 students can be encouraged to think about the implications of the problem solutions.

Chemical Engineering Departments

Departments are encouraged to consider adopting this book during the first introductory course in chemical engineering and then utilize 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 Accreditation Board for Engineering and Technology (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.

Educational Resources on CD-ROM

A CD-ROM is provided that contains additional learning resources including a complete operational version of the POLYMATH Numerical Computation Package which can be installed on a reader’s personal computer to enable efficient interactive problem solving. All illustrative solved problems are available from the CD-ROM for execution and modification using POLYMATH. Ten representative book problems have also been solved by knowledgeable professionals with Excel, Maple, Mathcad, Mathematica, MATLAB, and POLYMATH. Detailed writeups and the files to solve these problems with these packages are included on the CD-ROM. The icon at the beginning of this paragraph is used to designate a CD-ROM resource throughout the book. For many problems, tabulated data for individual problems are provided as input files to POLYMATH, thereby eliminating time-consuming data entry. The complete details on the CD-ROM are given in Appendix F.

Book Organization

Chapter 1, “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 introduces numerical solutions that are presented using the POLYMATH Numerical Computation Package. This material can also be used in a separate “Introduction to Personal Computers” course that can be given in parallel to the first chemical engineering course. For the past three years at Ben-Gurion University, the material from Chapter 1 of this book has been taught in the second semester of the first year, in parallel with the second part of the material and energy balance course. The students are introduced to the POLYMATH software in two two-hour lectures and two one-hour computer lab sessions. During the lectures and lab sessions, Problems 1.1, 1.3 and 1.13 are presented to introduce students to the different programs of POLYMATH. After this workshop, students are expected to use POLYMATH without additional help.

Chapters 2 and 3 are not associated with any particular required course in the chemical engineering curriculum. Chapter 2, “Regression and Correlation of Data,” presents advanced statistical techniques for regression of experimental data. Students can be encouraged to complete this chapter as part of a statistics course or as preparation for the chemical engineering laboratory. Chapter 3, “Advanced Techniques in Problem Solving,” provides the background necessary for solution of more complicated problems, such as stiff differential equations, two-point boundary value problems, and systems of differential-algebraic equations using interactive numerical software packages. This chapter can be integrated into the curriculum or covered as part of a separate numerical analysis course. The titles of the remaining chapters clearly indicate in which courses the problems can be used.

The fully or partially solved problems demonstrate solution methods that are not included in regular textbooks. Some of them also show advanced solution techniques that may not be obvious to the casual user. Table 3 lists these special techniques and the problem numbers in which they are demonstrated or required.

Book Notation

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. These books are summarized in Table 10.

The POLYMATH Numerical Computation Package

We have authored the POLYMATH package to provide convenient solutions to many numerical analysis problems, including the chemical engineering problems that are presented in this book.

The first PC version of POLYMATH was published in 1984, and it has been in use since then in over one hundred universities and selected industrial sites mainly in the United States and Israel. The initial version included with this book, POLYMATH 4.02, was released in May of 1998. This version executes in computers with DOS (and Windows) operating systems. The 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. No computer language is used, and a manual is not required. All problems can be stored on disk for future use. A sophisticated calculator and a general unit conversion utility are available from within POLYMATH upon request.

Current information on the latest POLYMATH software is available from http://www.polymath-software.com/.

Web Site: http://www.polymath-software.com/book

This site on the World Wide Web (WWW) will be maintained by the book authors to provide any corrections or updates to this book. The site will also provide information about where the CD-ROM may be reordered in the event that it has become damaged, outdated, or lost. Details on the latest POLYMATH software will also be available on the WWW, allowing inexpensive software upgrades to be downloaded. Additionally, the site may provide computer files for various solved problems for the convenient of readers to wish to use other mathematical software packages with this book.

Acknowledgments

We would like to express their 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. Numerical Analysis Package. We are indebted to our colleagues from the American Society for Engineering Education (ASEE) Chemical Engineering Summer School who permitted reproduction of their problem solutions on the CD-ROM. We thank Nancy Neborsky Pickering for initially learning the FrameMaker desktop publishing package and for entering the initial materials into the book format. Leslie Wang provided considerable valuable feedback on most chapters of the book. Additionally, we appreciate the input and suggestions of our students, who have been subjected to preliminary versions of the problems and have endured the various prerelease versions of the POLYMATH software over the years.

During the 17 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, H. S. Fogler, B. Carnahan, D. M. Himmelblau, J. D. Seader, and E. M. Rosen. H. S. Fogler and N. Brauner have also provided some of the problems included in the book and assisted with their solutions.

Development of a package such as POLYMATH and this book is an expensive endeavor in both resources and time. We are indebted to our universities: The Ben-Gurion University of the Negev and the University of Connecticut for the continuous support we have received. M. S. spent several summers and a sabbatical year at the University of Michigan. The first draft of this book was written during the stays at Michigan, and the support of the College of Engineering of the University of Michigan is sincerely appreciated. M. B. C. spent much of a sabbatical from the University of Connecticut and several summers on the preparation of book materials.

The routine maintenance and development of the POLYMATH package has been done by Orit Shacham. For the last 10 years she has been spending most of her vacations fixing bugs and writing new code for still another version of POLYMATH. She continues to amaze us by the speed and precision with which she converts ideas into computer code.

The first draft of 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 graphic programs and type the book. The draft she typed became the basis for class testing and refinement of the book.

Michael B. Cutlip
Mordechai Shacham

Table 1 Introductory Problems

NO.	INTRODUCTORY PROBLEMS
1.1	Molar Volume and Compressibility Factor from van der Waals Equation
1.2	Molar Volume and Compressibility Factor from Redlich-Kwong Equation
1.3	Fitting Polynomials and Correlation Equations to Vapor Pressure Data
1.4	Vapor Pressure Correlations for Sulfur Compounds Present in Petroleum
1.5	Steady-State Material Balances on a Separation Train
1.6	Mean Heat Capacity of *n*-Propane
1.7	Vapor Pressure Correlation by Clapeyron and Antoine Equations
1.8	Gas Volume Calculations Using Various Equations of State
1.9	Bubble Point Calculation for an Ideal Binary Mixture
1.10	Dew Point Calculation for an Ideal Binary Mixture
1.11	Bubble Point and Dew Point for an Ideal Multicomponent Mixture
1.12	Adiabatic Flame Temperature in Combustion
1.13	Unsteady-State Mixing in a Tank
1.14	Unsteady-State Mixing in a Series of Tanks
1.15	Heat Exchange in a Series of Tanks

Table 2 Problem in Regression and Correlation of Data

NO.	PROBLEMS IN REGRESSION AND CORRELATION OF DATA
2.1	Estimation of Antoine Equation Parameters Using Nonlinear Regression
2.2	Antoine Equation Parameters for Various Hydrocarbons
2.3	Correlation of Thermodynamic and Physical Properties of *n*-Propane
2.4	Temperature Dependency of Selected Properties
2.5	Heat Transfer Correlations from Dimensional Analysis
2.6	Heat Transfer Correlation of Liquids in Tubes
2.7	Heat Transfer Correlation in Fluidized Bed Reactor
2.8	Correlation of Binary Activity Coefficients Using Margules Equations
2.9	Margules Equations for Binary Systems Containing Trichloroethane
2.10	Rate Data Analysis for a Catalytic Reforming Reaction
2.11	Regression of Rate Data-Checking Dependency among Variables
2.12	Regression of Heterogeneous Catalytic Rate Data
2.13	Variation of Reaction Rate Constant with Temperature
2.14	Calculation of Antoine Equation Parameters Using Linear Regression
4.10	Correlation of Activity Coefficients with the van Laar Equations
8.7	Differential Method of Rate Data Analysis in a Batch Reactor
8.8	Integral Method of Rate Data Analysis in a Batch Reactor
8.9	Integral Method of Rate Data Analysis—Bimolecular Reaction
8.10	Initial Rate Method of Data Analysis
8.11	Half-Life Method for Rate Data Analysis
8.12	Method of Excess for Rate Data Analysis in a Batch Reactor
8.13	Rate Data Analysis for a CSTR
8.14	Differential Rate Data Analysis for a Plug-Flow Reactor
8.15	Integral Rate Data Analysis for a Plug-Flow Reactor
8.16	Rate Data Analysis for a Catalytic Reforming Reaction
8.17	Determination of Rate Expressions for a Catalytic Reaction

Table 3 Problem Solving Techniques

NO.	ADVANCED TECHNIQUES IN PROBLEM SOLVING
3.1	Demonstration of Iterative Methods for Solving a Nonlinear Equation (Terminal Velocity of Falling Particles)
3.2	Solution of Stiff Ordinary Differential Equations (A Biochemical Batch Reactor)
3.3	Stiff Ordinary Differential Equations in Chemical Kinetics (Gear's Stiff Problem in Chemical Kinetics)
3.4	Multiple Steady States in a System of ODEs (Transient Behavior of a Catalytic Fluidized Bed Reactor)
3.5	Single-Variable Optimization (Heat Transfer with Conduction and Radiation)
3.6	Shooting Method for Solving Two-Point Boundary Value Problems (Diffusion with First-Order Reaction in a Layer)
3.7	Expediting the Solution of Systems of Nonlinear Algebraic Equations (Complex Chemical Equilibrium)
3.8	Solving Differential Algebraic Equations (Binary Batch Distillation)
3.9	Method of Lines for Partial Differential Equations (Transient Heat Conduction in a Slab)

Table 4 Problems in Thermodynamics

NO.	PROBLEMS IN THERMODYNAMICS
1.1	Molar Volume and Compressibility Factor from van der Waals Equation
1.2	Molar Volume and Compressibility Factor from Redlich-Kwong Equation
1.3	Fitting Polynomials and Correlation Equations to Vapor Pressure Data
1.4	Vapor Pressure Correlations for Sulfur Compounds Present in Petroleum
1.6	Mean Heat Capacity of *n*-Propane
1.7	Vapor Pressure Correlation by Clapeyron and Antoine Equations
1.8	Gas Volume Calculations Using Various Equations of State
1.9	Bubble Point Calculation for an Ideal Binary Mixture
1.10	Dew Point Calculation for an Ideal Binary Mixture
1.11	Bubble Point and Dew Point for an Ideal Multicomponent Mixture
1.12	Adiabatic Flame Temperature in Combustion
2.1	Estimation of Antoine Equation Parameters Using Nonlinear Regression
2.2	Antoine Equation Parameters for Various Hydrocarbons
2.3	Correlation of Thermodynamic and Physical Properties of n-Propane
2.4	Temperature Dependency of Selected Properties
2.8	Correlation of Binary Activity Coefficients Using Margules Equations
2.14	Calculation of Antoine Equation Parameters Using Linear Regression
3.9	Expediting the Solution of Systems of Nonlinear Algebraic Equations (Equilibrium Problem)
4.1	Compressibility Factor Variation from van der Waals Equation
4.2	Compressibility Factor Variation from Various Equations of State
4.3	Isothermal Compression of Gas Using Redlich-Kwong Equation of State
4.4	Thermodynamic Properties of Steam from Redlich-Kwong Equation
4.5	Enthalpy and Entropy Departure Using the Redlich-Kwong Equation
4.6	Fugacity Coefficients of Pure Fluids from Various Equations of State
4.7	Fugacity Coefficients for Ammonia—Experimental and Predicted
4.8	Flash Evaporation of an Ideal Multicomponent Mixture
4.9	Flash Evaporation of Various Hydrocarbon Mixtures
4.10	Correlation of Activity Coefficients with the van Laar Equations
4.11	Vapor Liquid Equilibrium Data from Total Pressure Measurements I
4.12	Vapor Liquid Equilibrium Data from Total Pressure Measurements II

Table 4 Problems in Thermodynamics

NO.	PROBLEMS IN THERMODYNAMICS
4.13	Complex Chemical Equilibrium
4.14	Reaction Equilibrium at Constant Pressure or Constant Volume

Table 5 Problems in Fluid Mechanics

NO.	PROBLEMS IN FLUID MECHANICS
5.1	Laminar Flow of a Newtonian Fluid in a Horizontal Pipe
5.2	Laminar Flow of Non-Newtonian Fluids in a Horizontal Pipe
5.3	Vertical Laminar Flow of a Liquid Film
5.4	Laminar Flow of Non-Newtonian Fluids in a Horizontal Annulus
5.5	Temperature Dependency of Density and Viscosity of Various Liquids
5.6	Terminal Velocity of Falling Particles
5.7	Comparison of Friction Factor Correlations for Turbulent Pipe Flow
5.8	Calculations Involving Friction Factors for Flow in Pipes
5.9	Average Velocity in Turbulent Smooth Pipe Flow from Maximum Velocity
5.10	Calculation of the Flow Rate in a Pipeline
5.11	Flow Distribution in a Pipeline Network
5.12	Water Distribution Network
5.13	Pipe and Pump Network
5.14	Optimal Pipe Length for Draining a Cylindrical Tank in Turbulent Flow
5.15	Optimal Pipe Length for Draining a Cylindrical Tank in Laminar Flow
5.16	Baseball Trajectories as a Function of Elevation
5.17	Velocity Profiles for a Wall Suddenly Set in Motion—Laminar Flow
5.18	Boundary Layer Flow of a Newtonian Fluid on a Flat Plate
7.15	Diffusion into a Falling Laminar Liquid Film of Finite Thickness

Table 6 Problems in Heat Transfer

NO.	PROBLEMS IN HEAT TRANSFER
1.15	Heat Exchange in a Series of Tanks
3.5	Single Variable Optimization for a Heat Transfer Problem
3.9	Method of Lines for Unsteady State Heat Conduction in a Slab
6.1	One-Dimensional Heat Transfer through a Multilayered Wall
6.2	Heat Conduction in a Wire with Electrical Heat Source and Insulation
6.3	Radial Heat Transfer by Conduction with Convection at Boundaries
6.4	Energy Loss from an Insulated Pipe
6.5	Heat Loss through Pipe Flanges
6.6	Heat Transfer from a Horizontal Cylindrical Attached to a Heated Wall
6.7	Heat Transfer from a Triangular Fin
6.8	Single-Pass Heat Exchanger with Convective Heat Transfer on Tube Side
6.9	Double-Pipe Heat Exchanger
6.10	Heat Loss from an Uninsulated Tank Due to Convection
6.11	Unsteady-State Radiation to a Thin Plate
6.12	Unsteady-State Heat Conduction within a Semi-Infinite Slab
6.13	Cooling of a Solid Sphere in a Finite Water Bath
6.14	Unsteady-State Conduction in Two Dimensions
8.23	Material and Energy Balances on a Batch Reactor
8.24	Operation of a Cooled Exothermic CSTR
8.25	Exothermic Reversible Gas-Phase Reaction in a Packed Bed Reactor
8.26	Temperature Effects with Exothermic Reactions

Table 7 Problems in Mass Transfer

NO.	PROBLEMS IN MASS TRANSFER
3.6	Shooting Method for Solving Two-Point Boundary Problems
7.1	One-Dimensional Binary Mass Transfer in a Stefan Tube
7.2	Mass Transfer in a Packed Bed with Known Mass Transfer Coefficient
7.3	Slow Sublimation of a Solid Sphere
7.4	Controlled Drug Delivery by Dissolution of Pill Coating
7.5	Diffusion with Simultaneous Reaction in Isothermal Catalyst Particles
7.6	General Effectiveness Factor Calculations for First-Order Reactions
7.7	Simultaneous Diffusion and Reversible Reaction in a Catalytic Layer
7.8	Simultaneous Multicomponent Diffusion of Gases
7.9	Multicomponent Diffusion of Acetone and Methanol in Air
7.10	Multicomponent Diffusion in a Porous Layer Covering a Catalyst
7.11	Second-Order Reaction with Diffusion in Liquid Film
7.12	Simultaneous Heat and Mass Transfer in Catalyst Particles
7.13	Unsteady-State Mass Transfer in a Slab
7.14	Unsteady-State Diffusion and Reaction in a Semi-Infinite Slab
7.15	Diffusion into a Falling Laminar Liquid Film of Finite Thickness
8.4	Catalytic Reactor with Membrane Separation
8.27	Diffusion with Multiple Reactions in Porous Catalyst Particles

Table 8 Problems in Chemical Reaction Engineering

NO.	PROBLEMS IN CHEMICAL REACTION ENGINEERING
2.10	Rate Data Analysis for a Catalytic Reforming Reaction
2.11	Regression of Rate Data—Checking Dependency among Variables
2.12	Regression of Heterogeneous Catalytic Rate Data
2.13	Variation of Reaction Rate Constant with Temperature
3.6	Shooting Method for Solving Two-Point Boundary Value Problems (Diffusion with First-Order Reaction in a Layer)
4.13	Complex Chemical Equilibrium
4.14	Reaction Equilibrium at Constant Pressure or Constant Volume
8.1	Plug-Flow Reactor with Volume Change during Reaction
8.2	Variation of Conversion with Reaction Order in a Plug-Flow Reactor
8.3	Gas-Phase Reaction in a Packed Bed Reactor with Pressure Drop
8.4	Catalytic Reactor with Membrane Separation
8.5	Semibatch Reactor with Reversible Liquid-Phase Reaction
8.6	Operation of Three Continuous Stirred Tank Reactors in Series
8.7	Differential Method of Rate Data Analysis in a Batch Reactor
8.8	Integral Method of Rate Data Analysis in a Batch Reactor
8.9	Integral Method of Rate Data Analysis—Bimolecular Reaction
8.10	Initial Rate Method of Data Analysis
8.11	Half-Life Method for Rate Data Analysis
8.12	Method of Excess for Rate Data Analysis in a Batch Reactor
8.13	Rate Data Analysis for a CSTR
8.14	Differential Rate Data Analysis for a Plug-Flow Reactor
8.15	Integral Rate Data Analysis for a Plug-Flow Reactor
8.16	Rate Data Analysis for a Catalytic Reforming Reaction
8.17	Determination of Rate Expressions for a Catalytic Reaction
8.18	Packed Bed Reactor Design for a Gas-Phase Catalytic Reaction
8.19	Catalyst Decay in a Packed Bed Reactor Modeled by a Series of CSTRs
8.20	Design for Catalyst Decay in a Straight-Through Reactor
8.21	Enzymatic Reactions in a Batch Reactor
8.22	Isothermal Reactor Design for Multiple Reactions
8.23	Material and Energy Balances on a Batch Reactor

Table 8 Problems in Chemical Reaction Engineering

NO.	PROBLEMS IN CHEMICAL REACTION ENGINEERING
8.24	Operation of a Cooled Exothermic CSTR
8.25	Exothermic Reversible Gas-Phase Reaction in a Packed Bed Reactor
8.26	Temperature Effects with Exothermic Reactions
8.27	Diffusion with Multiple Reactions in Porous Catalyst Particles

Table 9 List of Advanced Solution Techniques Demonstrated in Various Problems

ADVANCED SOLUTION TECHNIQUES	PROBLEM NO.
Ordinary Differential Equations	
Plotting Solution Trajectory for an Algebraic Equation Using the ODE Solver	3.1, 4.1, 4.5
Solution of Stiff Differential Equations	3.2, 3.3, 3.4
Solution of Two-Point Boundary Value Problems by Shooting Methods	3.5, 3.6, 5.1, 5.2, 5.3, 5.4, 5.18, 6.2, 6.5, 6.6, 6.7, 7.1, 7.3, 7.5, 7.6, 7.7, 7.8, 7.9, 7.10, 7.12
Conversion of Higher-Order Differential Equations to System of First-Order ODEs	3.6, 5.16, 5.18, 6.2, 6.5
Solution of Differential Algebraic System of Equations	3.8
Using the l'Hôpital's Rule for Undefined Functions at the Beginning or End Point of Integration Interval	4.11, 4.12
Using "If" Statement to Avoid Division by Zero	5.1
Switching Variables On and Off during Integration	5.16
Retaining a Value when a Condition Is Satisfied	5.16
Generation of Error Function	5.17
Functions Undefined at the Initial Point	6.2, 6.5
Using "If" Statement to Match Different Equations to the Same Variable	6.2, 7.4
Implicit Finite Difference Techniques	7.7, 7.11
Partial Differential Equations	
Numerical Method of Lines	3.9, 5.17, 6.12, 6.13, 6.14, 7.13, 7.14, 7.15
Transformation to an ODE	5.18

Table 9 List of Advanced Solution Techniques Demonstrated in Various Problems

ADVANCED SOLUTION TECHNIQUES	PROBLEM NO.
Algebraic Equations	
Using "If" Statement to Match Different Equations to One Variable	3.1, 5.6, 5.10
Ill-Conditioned Systems	3.4
Conversion of a System of Nonlinear Equations into a Single Equation	3.4
Selection of Initial Estimates	3.6, 4.12, 7.2
Modification of Strongly Nonlinear Equations for Easier Solution	3.7, 4.13
Conversion of a Nonlinear Algebraic Equation to a Differential Equation	4.1, 4.2, 4.5, 4.6
Data Modeling and Analysis	
Using Residual Plot for Data Analysis	1.3, 1.4, 2.1, 2.3, 2.5, 2.8, 2.14, 4.10
Using Confidence Intervals for Checking Significance of Parameters	1.3, 1.4, 2.1, 2.3, 2.8, 4.10
Transformation of Nonlinear Models for Linear Representations	1.3, 2.3, 2.5, 2.8
Differentiation and Integration of Tabular Data	1.6, 8.7, 8.12, 8.14, 8.15
Checking Linear Dependency among Independent Variables	2.11
Comparison of Linear and Nonlinear Regression	2.12, 2.13, 8.7

Table 10 Prentice Hall Textbooks for Notation

Prentice Hall Textbooks	
Author	**Title**
Himmelblau[4]	*Basic Principles and Calculations in Chemical Engineering*
Kyle[6]	*Chemical and Process Thermodynamics*
Geankoplis[3]	*Transport Processes and Unit Operations*
Fogler[2]	*Elements of Chemical Reaction Engineering*

REFERENCES

1. deNevers, N.,and Seader, J.D. "Helping Students to Develop a Critical Attitude Towards Chemical Process Calculations", *Chem. Engr. Ed.*, 26 (2), pp. 88-93 (1992).
2. Fogler, H.S. Elements of Chemical Reaction Engineering, 2nd ed., Prentice Hall, Englewood Cliffs: NJ, 1992.
3. Geankoplis, C. J. *Transport Processes and Unit Operations*, 3rd ed, Englewood Cliffs, NJ: Prentice-Hall, 1993.
4. Himmelblau, D. M., *Basic Principles and Calculations in Chemical Engineering*, 6th ed, Englewood Cliffs, NJ: Prentice-Hall, 1996.
5. Jones, J. B. "The Non-Use of Computers in Undergraduate Engineering Science Courses", *J. Engr. Ed.*, 87(1), 11 (1998).
6. Kyle, B. G. *Chemical and Process Thermodynamics*, 2nd ed, Englewood Cliffs, NJ: Prentice-Hall, 1992.

APPENDIX F

The CD-ROM

Important resources on the CD-ROM for use with this book that are available on the accompanying CD-ROM include:

1. Polymath software for installation to a personal computer operating under DOS, Windows 3.1, Windows 95, and Windows NT.
2. Acrobat* PDF software for installation to a personal computer operating under Windows 3.1, Windows 95, and Windows NT. Acrobat software 3.0 and above is necessary to view and print the enclosed documents in PDF format using most any computer, operating system, and printer.
3. Polymath manual in Adobe Acrobat PDF format.
4. Polymath solutions or data for selected problems as referenced in the book.
5. Polymath data sets for selected tables for use in problem solving.
6. A set of ten representative problems in Chemical Engineering with detailed writeups and problem code for execution by various mathematical software packages. Documentation is in Adobe Acrobat PDF format. Packages include Excel, Maple, Mathcad, MATLAB, Mathematica, and POLYMATH.
7. Description of the POLYMATH software in PDF format.
8. Information on updating of book material in PDF format.
9. Information on updating of POLYMATH software in PDF format.
10. Information on updating of Acrobat software in PDF format.

Using the CD-ROM

The CD that accompanied this book is organized just like any typical hard disk. CD hardware is typically given a drive letter when it is installed into a computer. **All further discussion of the CD will assume that the CD is called drive D**. The software on the CD is provided in subdirectories of drive D that are identified in the following descriptions. It is recommended that the software be installed in the order as discussed since both POLYMATH and the Adobe Acrobat Reader software are essential to the use of the CD-ROM.

* Acrobat is a trademark of Adobe Systems, Inc. (http://www.adobe.com)

Installation of POLYMATH Software to a Personal Computer

The POLYMATH software must be installed to a hard disk drive. The details of this installation are provided on the file called INSTALL.TXT. This file should be printed and referenced during the installation process. This can be accomplished with utility software such as Notepad or with word processing packages such as WordPerfect and Microsoft Word.

The POLYMATH software package and associated files are found in D:\POLYMATH. The INSTALL.TXT file gives the essentials of installation while the README.TXT file gives more information on POLYMATH and the License Agreement. The installation is initiated by executing the file INSTALL.EXE from this subdirectory.

Installation of Adobe Acrobat Reader Software to a Personal Computer

The Adobe Acrobat Reader software must also be installed to a hard disk. This software will allow you to read and print additional materials that are on the CD-ROM. This software is also freely available by downloading from www.adobe.com for many different operating systems.

The Adobe Acrobat Reader software is found in D:\ADOBE. The following files should be executed from the CD-ROM according to your operating system. The installation is self-documented and completely automatic. Use the following:

AR32E301.EXE for Windows 95 and Windows NT

AR16E301.EXE for Windows 3.1.

Accessing the POLYMATH Manual

The POLYMATH Manual is available as a. Adobe Acrobat PDF file found in the directory D:\MANUAL with file name MANUAL.PDF. From Adobe Acrobat, just open this file from the CD-ROM to view or print the manual. You may also search on words or terms of interest using Acrobat.

Learning to Use the POLYMATH Software

The POLYMATH software package is very user-friendly and menu-driven so that it is very easy to use. First-time computer users should make a hard copy of the manual as indicated above. The manual will be a convenient reference guide when using POLYMATH. Then it will be helpful to read through the manual and try many of the QUICK TOUR problems. If you have considerable computer experience, you only need to read the chapters at the back of the manual that discuss the individual programs of interest to you and try some of the QUICK TOUR problems.

Particular attention should be directed at the sections which describe the Library Operations, Library Storage and Library Retrieval as these options are used to provide solutions to many of the problems in this book. These options also allow users to conveniently store their problems for future use. Each POLY-

MATH program will only show the problems in a particular Library which are relevant to that program. For example, a particular Library when accessed from POLYMATH Simultaneous Differential Equation Solver will only indicate those problems that can be solved with that package when there may be many other problems in the same Library for all other POLYMATH programs.

Accessing the POLYMATH Solutions of Selected Problems

Selected problems in this book contain partial or complete solutions using POLYMATH. These solutions are provided on the CD-ROM by using the POLYMATH Library options. This enables the user to retrieve the problem from a particular Library on the CD-ROM and execute the problem within POLYMATH. It is important to note that the Library stores only the problem and not the solution; however, it is a simple matter to solve the particular problem with POLYMATH. The solved problem can then be examined with the various plotting and tabular data options, and the problem can easily be modified prior to another solution. Printing of intermediate and final results is quite easy. The interactive nature of POLYMATH greatly enhances the problem-solving experience. The Library option can to used to store problems as desired.

The solved problems associated with the book are stored on the CD-ROM using the Library in directories D:\CHAP1 ... CHAP8. Identification of the particular POLYMATH program and the Library location is given in each problem.

Accessing the POLYMATH Data Sets for Selected Tables

Selected tables in the chapters and in the appendices have been entered into the POLYMATH *Polynomial, Multiple Linear and Nonlinear Regression Program*. These tables of data can be loaded from the identified Library for use in problem solving so that the user can easily utilize the original data set without data entry.

The selected tables associated with the book are stored on the CD-ROM using the Library in directory D:\TABLES. Identification of the particular table file is by the table number and title used in the book.

Using the Set of Ten Problems in Chemical Engineering with Other Mathematical Solving Software

While POLYMATH is used to demonstrate numerical problem-solving throughout this book, a number of other mathematical software packages can be utilized to solve these same problems.

The use of mathematical software in chemical engineering was the subject of session at a conference sponsored by the Chemical Engineering Division of the American Society for Engineering Education*. This session presented solutions

* The original materials were distributed at the Chemical Engineering Summer School at Snowbird, Utah on August 13, 1997 in Session 12 entitled "The Use of Mathematical Software in Chemical Engineering."

to ten representative problems in chemical engineering which were solved by different mathematical packages. The papers from this session were enhanced to include detailed solutions papers that utilized Excel[*], Maple[†], Mathcad[‡], MATLAB[•], Mathematica[#], and POLYMATH[¶]. An article based on this problem set and the various solutions is to be published in *Computer Applications in Engineering Education*[**]. The contributing authors were:

Excel - Edward M. Rosen, EMR Technology Group

Maple - Ross Taylor, Clarkson University

MathCAD - John J. Hwalek, University of Maine

MATLAB - Joseph Brule, John Widmann, Tae Han, and Bruce Finlayson, University of Washington

Mathematica - H. Eric Nuttall, University of New Mexico

POLYMATH - Michael B. Cutlip, University of Connecticut and Mordechai Shacham, Ben-Gurion University of the Negev

Many of these ten problems are also problems in this book since the book authors were the organizers and participants in the ASEE session. The authors of these materials have kindly permitted the inclusion of the ten problems paper and the detailed solution manuscripts as PDF files on the CD-ROM. Additionally, the computer files are also available on the CD-ROM so that these problem solutions can be executed by using the appropriate software package.

A summary of the ten problems and the corresponding numbering to the problems in this book is given in Table F–1. Individuals who prefer to use one of these various mathematical software packages will find the detailed writeups and problem files very helpful in utilizing these packages.

The paper entitled “A Collection of Representative Problems in Chemical Engineering for Solution by Numerical Methods” is found in directory D:\TENPROBS with file named TENPROBS.PDF. The various papers discussing the solutions are located in individual subdirectories with the name of that software package. For example, the Maple paper is found in D:\TENPROBS\MAPLE with the file named MAPLE.PDF. Individual solution files are found in a subdirectory below each package directory such as D:\TENPROBS\MATHCAD with files named PROBLEM1.MCD... PROBLEM10.MCD.

[*] Excel is a trademark of Microsoft Corporation (http://www.microsoft.com)
[†] Maple is a trademark of Waterloo Maple, Inc. (http://www.maplesoft.com)
[‡] MathCAD is a trademark of Mathsoft, Inc. (http://www.mathsoft.com)
[•] MATLAB is a trademark of The Math Works, Inc. (http://www.mathworks.com)
[#] Mathematica is a trademark of Wolfram Research, Inc. (http://www.wolfram.com)
[¶] POLYMATH is copyrighted by M. Shacham and M. B. Cutlip (http://www.polymath-software.com)
[**] The Journal *Computer Applications in Engineering Education* is published by John Wiley & Sons, Inc., and the editor is M. F. Iskander. (http://www.journals.wiley.com/1061-3773)

Table F–1 Ten Representative Problem in Chemical Engineering

SUBJECT AREA	PROBLEM TITLE	MATHEMATICAL MODEL	ORIGINAL PROBLEM	THIS BOOK PROBLEM
Introduction to Ch. E.	Molar Volume and Compressibility Factor from Van Der Waals Equation	Single Nonlinear Equation	1	1.1
Introduction to Ch. E.	Steady State Material Balances on a Separation Train	Simultaneous Linear Equations	2	1.5
Mathematical Methods	Vapor Pressure Data Representation by Polynomials and Equations	Polynomial Fitting, Linear and Nonlinear Regression	3	1.3 and 2.1
Thermodynamics	Reaction Equilibrium for Multiple Gas Phase Reactions	Simultaneous Nonlinear Equations	4	4.13
Fluid Dynamics	Terminal Velocity of Falling Particles	Single Nonlinear Equation	5	5.6
Heat Transfer	Unsteady State Heat Exchange in a Series of Agitated Tanks	Simultaneous ODE's with known initial conditions.	6	1.15
Mass Transfer	Diffusion with Chemical Reaction in a One Dimensional Slab	Simultaneous ODE's with split boundary conditions.	7	3.6
Separation Processes	Binary Batch Distillation	Simultaneous Differential and Nonlinear Algebraic Equations	8	3.8
Reaction Engineering	Reversible, Exothermic, Gas Phase Reaction in a Catalytic Reactor	Simultaneous ODE's and Algebraic Equations	9	8.24
Process Dynamics and Control	Dynamics of a Heated Tank with PI Temperature Control	Simultaneous Stiff ODE's	10	-

TREE STRUCTURE OF THE CD-ROM

Figure F–1 indicates the tree structure of the CD-ROM.

TECHNICAL SUPPORT FOR THE CD-ROM

Technical support for this CD-ROM is available at (800)842-2958.

UPDATING THE BOOK AND OTHER CD-ROM MATERIALS

Corrections and additions to the book content will be avilable via the Internet at www.polymath-software.com/book. The latest description and information on the POLYMATH Numerical Analysis Package is provided at www.polymath-software.com. Details and downloading information on the Adobe Acrobat software is found at www.adobe.com.

Updating information is also on the CD-ROM in directory D:\UPDATE with files named BOOK.PDF, POLYMATH.PDF, and ADOBE.PDF.

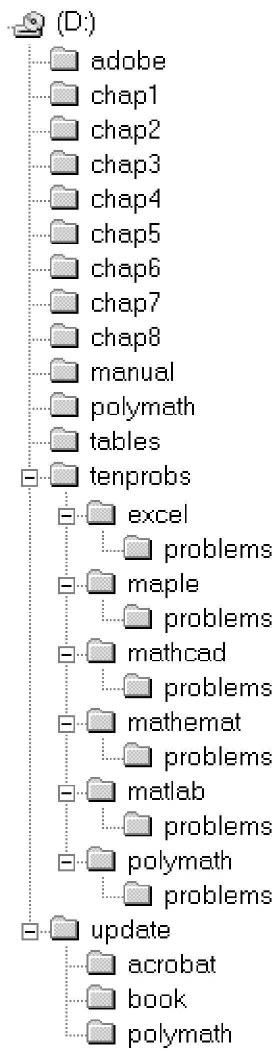

Figure F–1 Directory Tree Structure for CD-ROM

Numerical Methods and Modeling. for Chemical Engineers. Initlal..Value Problems for Ordinary Differential Equations. INTRODUCTION. The goal of this book is to expose the reader to modern computational tools for solving differential equation models that arise in chemical engineering, e.g., diffusion-reaction, mass-heat transfer, and fluid flow.Â Many problems in engineering and science can be formulated in terms of dif-ferential equations. A differential equation is an equation involving a relation between an unknown function and one or more of its derivatives. Equations involving derivatives of only one independent variable are called ordinary dif-ferential equations and may be classified as either initial-value problems (IVP) or boundary-value problems (BVP). The Runge-Kutta Method is a commonly used numerical method for solving 1st-order ordinary differential equations (ODEs) with a known initial condition. The method starts at a known point and develops the solution to the ODE by proceeding stepwise in small increments. ï,· ï,· It is used to solve Variable Volume/Concentration Tank Problem Used to check the set of equations for absorber calculation.Â Two cases of typical problems in chemical engineering, that result in a variety of forms Case I. A chemical equilibrium problem Case II. AJash distillation problem. Application of Taylor Series method in chemical engineering Taylor series is a representation of a function as an infinite sum of terms that are calculated from the values of the function's derivatives at a single point.