Contents

List of Illustrations xi
List of Tables xvi
List of Programs xvii
Preface xix
Acknowledgments xxiv

1 Mathematical Modeling and Structured Programming 1
1.1 Elements of a Mathematical Model 1
1.2 Some Analytically Solvable Chemical Engineering Models 4
   1.2.1 Vapor–Liquid Equilibrium 4
   1.2.2 Batch Reactor with a Single Reactant 6
   1.2.3 Batch Reactor with Three Species 8
   1.2.4 Continuous Stirred Tank Reactor 12
   1.2.5 Reaction–Diffusion in a Slab 13
   1.2.6 Unsteady Diffusion 15
1.3 Computer Math 20
   1.3.1 Three Key Operations 20
   1.3.2 Words and Round-Off Error 22
1.4 Structured Programming 23
   1.4.1 Learning to Program 24
   1.4.2 The for Loop 25
   1.4.3 The while Loop 28
   1.4.4 If-else Statements 30
   1.4.5 Modular Programming 33
1.5 Further Reading 35
Problems 35
Computer Problems 41

2 Linear Algebraic Equations 45
2.1 Definition of a Linear System of Algebraic Equations 45
2.2 Does a Solution Exist? 47
2.3 Conditioning 48
   2.3.1 Vector Spaces 49
## Contents

2.3.2 Vector Norms 51  
2.3.3 Matrix Norms 52  
2.3.4 Condition Number 53  
2.4 Cramer’s Rule 56  
2.5 Gauss Elimination 58  
  2.5.1 Algorithm 60  
  2.5.2 Computational Cost 64  
2.6 Pivoting 66  
  2.6.1 A Simple Example 66  
  2.6.2 Algorithm 68  
2.7 Case Study: Multi-component Flash 72  
  2.7.1 Problem Statement 72  
  2.7.2 Solution 73  
2.8 Calculation of the Determinant by Gauss Elimination 78  
2.9 Banded Matrices 80  
2.10 Simultaneous Gauss Elimination 82  
2.11 LU Decomposition 83  
  2.11.1 Doolittle’s Method 84  
  2.11.2 Implementation 89  
2.12 Case Study: Linear Process Flow Sheet 91  
  2.12.1 Problem Statement 91  
  2.12.2 Solution 92  
2.13 Iterative Methods 95  
  2.13.1 Jacobi’s Method 96  
  2.13.2 Gauss–Seidel Method 100  
  2.13.3 Successive Relaxation Method 103  
  2.13.4 Convergence 105  
2.14 Application: Polynomial Regression 107  
2.15 Implementation in MATLAB 112  
2.16 Further Reading 114  
Problems 116  
Computer Problems 132  

### 3 Nonlinear Algebraic Equations

3.1 Introduction 136  
  3.1.1 Superposition 137  
  3.1.2 Differences Between Linear and Nonlinear Equations 138  
3.2 Solution Approaches 140  
  3.2.1 Bracketing Methods 141  
  3.2.2 Fixed-Point (Open) Methods 143  
3.3 Fixed-Point Methods for Single Nonlinear Algebraic Equations 145  
  3.3.1 Picard’s Method 146  
  3.3.2 Newton’s Method 148  
3.4 Convergence of General Fixed-Point Iteration 152
## Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4.1 Will We Find a Solution?</td>
<td>153</td>
</tr>
<tr>
<td>3.4.2 Rate of Convergence</td>
<td>156</td>
</tr>
<tr>
<td>3.5 Case Study: Eigenvalue Calculation in Unsteady Diffusion</td>
<td>158</td>
</tr>
<tr>
<td>3.5.1 Problem Statement</td>
<td>158</td>
</tr>
<tr>
<td>3.5.2 Solution</td>
<td>159</td>
</tr>
<tr>
<td>3.6 Case Study: Extension of a Tethered Polymer by a Force</td>
<td>160</td>
</tr>
<tr>
<td>3.6.1 Problem Statement</td>
<td>160</td>
</tr>
<tr>
<td>3.6.2 Solution</td>
<td>162</td>
</tr>
<tr>
<td>3.7 Systems of Nonlinear Algebraic Equations</td>
<td>164</td>
</tr>
<tr>
<td>3.7.1 Picard’s Method</td>
<td>165</td>
</tr>
<tr>
<td>3.7.2 Newton–Raphson</td>
<td>167</td>
</tr>
<tr>
<td>3.8 Case Study: Nonlinear Flash</td>
<td>177</td>
</tr>
<tr>
<td>3.8.1 Problem Statement</td>
<td>177</td>
</tr>
<tr>
<td>3.8.2 Solution</td>
<td>177</td>
</tr>
<tr>
<td>3.8.3 A Variation on the Problem</td>
<td>179</td>
</tr>
<tr>
<td>3.9 Continuation Methods</td>
<td>180</td>
</tr>
<tr>
<td>3.9.1 Zero-Order Continuation</td>
<td>181</td>
</tr>
<tr>
<td>3.9.2 First-Order Continuation</td>
<td>181</td>
</tr>
<tr>
<td>3.10 Case Study: Liquid–Liquid Phase Diagram from the van Laar Model</td>
<td>182</td>
</tr>
<tr>
<td>3.10.1 Problem Statement</td>
<td>182</td>
</tr>
<tr>
<td>3.10.2 Solution</td>
<td>183</td>
</tr>
<tr>
<td>3.11 Implementation in MATLAB</td>
<td>188</td>
</tr>
<tr>
<td>3.12 Further Reading</td>
<td>190</td>
</tr>
<tr>
<td>Problems</td>
<td>191</td>
</tr>
<tr>
<td>Computer Problems</td>
<td>195</td>
</tr>
<tr>
<td>4 Initial Value Problems</td>
<td>206</td>
</tr>
<tr>
<td>4.1 Introduction</td>
<td>206</td>
</tr>
<tr>
<td>4.1.1 Classification of ODE Problems</td>
<td>206</td>
</tr>
<tr>
<td>4.1.2 General Solution Approach</td>
<td>208</td>
</tr>
<tr>
<td>4.2 First-Order ODE IVPs</td>
<td>208</td>
</tr>
<tr>
<td>4.2.1 Explicit (Forward) Euler</td>
<td>209</td>
</tr>
<tr>
<td>4.2.2 Implicit (Backward) Euler</td>
<td>214</td>
</tr>
<tr>
<td>4.2.3 Predictor–Corrector</td>
<td>220</td>
</tr>
<tr>
<td>4.2.4 Runge–Kutta Methods</td>
<td>221</td>
</tr>
<tr>
<td>4.3 Numerical Stability</td>
<td>228</td>
</tr>
<tr>
<td>4.3.1 Linear IVPs</td>
<td>229</td>
</tr>
<tr>
<td>4.3.2 Nonlinear IVPs</td>
<td>232</td>
</tr>
<tr>
<td>4.4 Case Study: CSTR with a Fluctuating Inlet</td>
<td>232</td>
</tr>
<tr>
<td>4.4.1 Problem Statement</td>
<td>232</td>
</tr>
<tr>
<td>4.4.2 Solution</td>
<td>233</td>
</tr>
<tr>
<td>4.5 Case Study: Liquid Level Dynamics and Control</td>
<td>236</td>
</tr>
<tr>
<td>4.5.1 Problem Statement</td>
<td>236</td>
</tr>
<tr>
<td>4.5.2 Solution</td>
<td>238</td>
</tr>
</tbody>
</table>
4.6 Systems of ODE IVPs
4.6.1 Explicit Methods
4.6.2 Implicit Euler
4.7 Higher-Order ODE Euler
4.8 Numerical Stability for Systems of ODEs
4.8.1 Analysis by Matrix Diagonalization
4.8.2 Stiff Systems
4.9 Case Study: Non-Isothermal PFR
4.9.1 Problem Statement
4.9.2 Solution
4.10 Implementation in MATLAB
4.11 Further Reading

Problems
Computer Problems

5 Dynamical Systems
5.1 Introduction
5.2 Equilibrium Points and Their Stability
5.3 Dynamical Systems on the Plane
5.3.1 Linear Systems on the Plane – Classification of Steady States
5.3.2 Nonlinear Systems on the Plane
5.4 Nonlinear Phenomena
5.4.1 Periodic Solutions
5.4.2 Limit Cycles
5.5 Bifurcations
5.5.1 One-Dimensional Systems
5.5.2 Two-Dimensional Systems
5.6 Deterministic Chaos
5.7 Case Study: Non-Isothermal CSTR
5.7.1 Problem Statement
5.7.2 Solution
5.8 Implementation in MATLAB
5.9 Further Reading

Problems
Computer Problems

6 Boundary Value Problems
6.1 ODE Boundary Value Problems
6.2 Finite Difference Approximations
6.2.1 Discretization in Space
6.2.2 Derivation of Finite Difference Equations
6.3 Solution Procedure
6.3.1 Dirichlet Boundary Conditions
6.3.2 Neumann and Robin Boundary Conditions
### Table of Contents

6.3.3 Position-Dependent Terms 344  
6.3.4 Mesh Refinement 348  
6.4 Case Study: Reaction–Diffusion in a Packed Bed 352  
6.4.1 Problem Statement 352  
6.4.2 Solution 353  
6.5 Coupled BVPs 355  
6.5.1 Approach #1:Appending the Unknown Vectors 356  
6.5.2 Approach #2:Interlacing the Variables 357  
6.6 Case Study: Coupled Heat and Mass Transfer 358  
6.6.1 Problem Statement 358  
6.6.2 Solution 359  
6.7 Implementation in MATLAB 366  
6.8 Further Reading 366  
Problems 366  
Computer Problems 368

7 Partial Differential Equations 374  
7.1 Introduction 374  
7.2 Solution of IBVPs – Method of Lines 375  
7.2.1 Solution Method 376  
7.2.2 Numerical Stability 379  
7.3 Case Study: Unsteady Diffusion Through a Membrane 386  
7.3.1 Problem Statement 386  
7.3.2 Solution 388  
7.4 Two-Dimensional BVPs 392  
7.5 Case Study: 2D Reaction–Diffusion 401  
7.5.1 Problem Statement 401  
7.5.2 Solution 402  
7.6 Implementation in MATLAB 408  
7.7 Further Reading 409  
Problems 409  
Computer Problems 413

8 Interpolation and Integration 421  
8.1 Introduction 421  
8.2 Polynomial Interpolation 422  
8.2.1 Linear Interpolation 422  
8.2.2 Quadratic Interpolation 423  
8.2.3 Newton’s Divided Differences and Polynomial Interpolation 425  
8.2.4 Equally Spaced Data 431  
8.2.5 Error of Newton’s Interpolating Polynomials 433  
8.3 Newton–Coates Integration 434  
8.3.1 Trapezoidal Rule ($n = 1$) 435  
8.3.2 Simpson’s $1/3$ Rule ($n = 2$) 436
Contents

8.3.3 Higher-Order Formulas 437
8.4 Applications of Trapezoidal Rule 439
8.4.1 Multiple Trapezoidal Rule 439
8.4.2 Richardson Extrapolation 442
8.4.3 Romberg Integration 444
8.5 Gauss Quadrature 447
8.6 Case Study: Concentrated Differential Distillation 451
8.6.1 Problem Statement 451
8.6.2 Solution 453
8.7 Implementation in MATLAB 455
8.8 Further Reading 456
Problems 456
Computer Problems 458

Appendix A MATLAB “Tutorial” 464
A.1 Data Structures 464
A.2 Matrix and Vector Manipulation 468
A.3 Order of Operations 472
A.4 Displaying Data on the Screen 473
A.5 Logical Flow 474
A.6 Loops 476
A.7 Plotting 477
A.8 Functions 479

Appendix B Determinant of a Matrix 482

Index 486