

Contents

Chapter 1	Formulation of Physicochemical Problems	3
1.1	Introduction	3
1.2	Illustration of the Formulation Process (Cooling of Fluids)	4
1.3	Combining Rate and Equilibrium Concepts (Packed Bed Adsorber)	10
1.4	Boundary Conditions and Sign Conventions	13
1.5	Summary of the Model Building Process	16
1.6	Model Hierarchy and Its Importance in Analysis	17
1.7	References	28
1.8	Problems	28
Chapter 2	Solution Techniques for Models Yielding Ordinary Differential Equations (ODE)	37
2.1	Geometric Basis and Functionality	37
2.2	Classification of ODE	39
2.3	First Order Equations	39
2.3.1	Exact Solutions	41
2.3.2	Equations Composed of Homogeneous Functions	43
2.3.3	Bernoulli's Equation	45
2.3.4	Riccati's Equation	45
2.3.5	Linear Coefficients	49
2.3.6	First Order Equations of Second Degree	50
2.4	Solution Methods for Second Order Nonlinear Equations	51
2.4.1	Derivative Substitution Method	52
2.4.2	Homogeneous Function Method	58
2.5	Linear Equations of Higher Order	61
2.5.1	Second Order Unforced Equations: Complementary Solutions	63
2.5.2	Particular Solution Methods for Forced Equations	72
2.5.3	Summary of Particular Solution Methods	88
2.6	Coupled Simultaneous ODE	89
2.7	Summary of Solution Methods for ODE	96
2.8	References	97
2.9	Problems	97

Chapter 3	Series Solution Methods and Special Functions	104
3.1	Introduction to Series Methods	104
3.2	Properties of Infinite Series	106
3.3	Method of Frobenius	108
3.3.1	Indicial Equation and Recurrence Relation	109
3.4	Summary of the Frobenius Method	126
3.5	Special Functions	127
3.5.1	Bessel's Equation	128
3.5.2	Modified Bessel's Equation	130
3.5.3	Generalized Bessel Equation	131
3.5.4	Properties of Bessel Functions	135
3.5.5	Differential, Integral and Recurrence Relations	137
3.6	References	141
3.7	Problems	142
Chapter 4	Integral Functions	148
4.1	Introduction	148
4.2	The Error Function	148
4.2.1	Properties of Error Function	149
4.3	The Gamma and Beta Functions	150
4.3.1	The Gamma Function	150
4.3.2	The Beta Function	152
4.4	The Elliptic Integrals	152
4.5	The Exponential and Trigonometric Integrals	156
4.6	References	158
4.7	Problems	158
Chapter 5	Staged-Process Models: The Calculus of Finite Differences	164
5.1	Introduction	164
5.1.1	Modeling Multiple Stages	165
5.2	Solution Methods for Linear Finite Difference Equations	166
5.2.1	Complementary Solutions	167
5.3	Particular Solution Methods	172
5.3.1	Method of Undetermined Coefficients	172
5.3.2	Inverse Operator Method	174
5.4	Nonlinear Equations (Riccati Equation)	176
5.5	References	179
5.6	Problems	179
Chapter 6	Approximate Solution Methods for ODE: Perturbation Methods	184
6.1	Perturbation Methods	184
6.1.1	Introduction	184
6.2	The Basic Concepts	189
6.2.1	Gauge Functions	189
6.2.2	Order Symbols	190
6.2.3	Asymptotic Expansions and Sequences	191
6.2.4	Sources of Nonuniformity	193

6.3	The Method of Matched Asymptotic Expansion	195
6.3.1	Matched Asymptotic Expansions for Coupled Equations	202
6.4	References	207
6.5	Problems	208

Chapter 7 Numerical Solution Methods (Initial Value Problems) 225

7.1	Introduction	225
7.2	Type of Method	230
7.3	Stability	232
7.4	Stiffness	243
7.5	Interpolation and Quadrature	246
7.6	Explicit Integration Methods	249
7.7	Implicit Integration Methods	252
7.8	Predictor-Corrector Methods and Runge-Kutta Methods	253
7.8.1	Predictor-Corrector Methods	253
7.8.2	Runge-Kutta Methods	254
7.9	Extrapolation	258
7.10	Step Size Control	258
7.11	Higher Order Integration Methods	260
7.12	References	260
7.13	Problems	261

Chapter 8 Approximate Methods for Boundary Value Problems: Weighted Residuals 268

8.1	The Method of Weighted Residuals	268
8.1.1	Variations on a Theme of Weighted Residuals	271
8.2	Jacobi Polynomials	285
8.2.1	Rodrigues Formula	285
8.2.2	Orthogonality Conditions	286
8.3	Lagrange Interpolation Polynomials	289
8.4	Orthogonal Collocation Method	290
8.4.1	Differentiation of a Lagrange Interpolation Polynomial	291
8.4.2	Gauss-Jacobi Quadrature	293
8.4.3	Radau and Lobatto Quadrature	295
8.5	Linear Boundary Value Problem— Dirichlet Boundary Condition	296
8.6	Linear Boundary Value Problem— Robin Boundary Condition	301
8.7	Nonlinear Boundary Value Problem— Dirichlet Boundary Condition	304
8.8	One-Point Collocation	309
8.9	Summary of Collocation Methods	311
8.10	Concluding Remarks	313
8.11	References	313
8.12	Problems	314

Chapter 9	Introduction to Complex Variables and Laplace Transforms	331
9.1	Introduction	331
9.2	Elements of Complex Variables	332
9.3	Elementary Functions of Complex Variables	334
9.4	Multivalued Functions	335
9.5	Continuity Properties for Complex Variables: Analyticity	337
9.5.1	Exploiting Singularities	341
9.6	Integration: Cauchy's Theorem	341
9.7	Cauchy's Theory of Residues	345
9.7.1	Practical Evaluation of Residues	347
9.7.2	Residues at Multiple Poles	349
9.8	Inversion of Laplace Transforms by Contour Integration	350
9.8.1	Summary of Inversion Theorem for Pole Singularities	353
9.9	Laplace Transformations: Building Blocks	354
9.9.1	Taking the Transform	354
9.9.2	Transforms of Derivatives and Integrals	357
9.9.3	The Shifting Theorem	360
9.9.4	Transform of Distribution Functions	361
9.10	Practical Inversion Methods	363
9.10.1	Partial Fractions	363
9.10.2	Convolution Theorem	366
9.11	Applications of Laplace Transforms for Solutions of ODE	368
9.12	Inversion Theory for Multivalued Functions: The Second Bromwich Path	378
9.12.1	Inversion when Poles and Branch Points Exist	382
9.13	Numerical Inversion Techniques	383
9.13.1	The Zakian Method	383
9.13.2	The Fourier Series Approximation	388
9.14	References	390
9.15	Problems	390
Chapter 10	Solution Techniques for Models Producing PDEs	397
10.1	Introduction	397
10.1.1	Classification and Characteristics of Linear Equations	402
10.2	Particular Solutions for PDEs	405
10.2.1	Boundary and Initial Conditions	406
10.3	Combination of Variables Method	409
10.4	Separation of Variables Method	420
10.4.1	Coated Wall Reactor	421
10.5	Orthogonal Functions and Sturm–Liouville Conditions	426
10.5.1	The Sturm–Liouville Equation	426
10.6	Inhomogeneous Equations	434
10.7	Applications of Laplace Transforms for Solutions of PDEs	443
10.8	References	454
10.9	Problems	455

Chapter 11	Transform Methods for Linear PDEs	486
11.1	Introduction	486
11.2	Transforms in Finite Domain: Sturm–Liouville Transforms	487
11.2.1	Development of Integral Transform Pairs	487
11.2.2	The Eigenvalue Problem and the Orthogonality Condition	494
11.2.3	Inhomogeneous Boundary Conditions	504
11.2.4	Inhomogeneous Equations	511
11.2.5	Time-Dependent Boundary Conditions	513
11.2.6	Elliptic Partial Differential Equations	516
11.3	Generalized Sturm–Liouville Integral Transform	521
11.3.1	Introduction	521
11.3.2	The Batch Adsorber Problem	521
11.4	References	537
11.5	Problems	538
Chapter 12	Approximate and Numerical Solution Methods for PDEs	546
12.1	Polynomial Approximation	546
12.2	Singular Perturbation	562
12.3	Finite Difference	572
12.3.1	Notations	573
12.3.2	Essence of the Method	574
12.3.3	Tridiagonal Matrix and the Thomas Algorithm	576
12.3.4	Linear Parabolic Partial Differential Equations	578
12.3.5	Nonlinear Parabolic Partial Differential Equations	586
12.3.6	Elliptic Equations	588
12.4	Orthogonal Collocation for Solving PDEs	592
12.4.1	Elliptic PDE	592
12.4.2	Parabolic PDE: Example 1	598
12.4.3	Coupled Parabolic PDE: Example 2	600
12.5	Orthogonal Collocation on Finite Elements	603
12.6	References	615
12.7	Problems	616
Appendix A:	Review of Methods for Nonlinear Algebraic Equations	630
A.1	The Bisection Algorithm	630
A.2	The Successive Substitution Method	632
A.3	The Newton–Raphson Method	635
A.4	Rate of Convergence	639
A.5	Multiplicity	641
A.6	Accelerating Convergence	642
A.7	References	643
Appendix B:	Vectors and Matrices	644
B.1	Matrix Definition	644
B.2	Types of Matrices	646
B.3	Matrix Algebra	647

B.4	Useful Row Operations	649
B.5	Direct Elimination Methods	651
B.5.1	Basic Procedure	651
B.5.2	Augmented Matrix	652
B.5.3	Pivoting	654
B.5.4	Scaling	655
B.5.5	Gauss Elimination	656
B.5.6	Gauss–Jordan Elimination	656
B.5.7	LU Decomposition	658
B.6	Iterative Methods	659
B.6.1	Jacobi Method	659
B.6.2	Gauss–Seidel Iteration Method	660
B.6.3	Successive Overrelaxation Method	660
B.7	Eigenproblems	660
B.8	Coupled Linear Differential Equations	661
B.9	References	662
Appendix C: Derivation of the Fourier–Mellin Inversion Theorem		663
Appendix D: Table of Laplace Transforms		671
Appendix E: Numerical Integration		676
E.1	Basic Idea of Numerical Integration	676
E.2	Newton Forward Difference Polynomial	677
E.3	Basic Integration Procedure	678
E.3.1	Trapezoid Rule	678
E.3.2	Simpson’s Rule	680
E.4	Error Control and Extrapolation	682
E.5	Gaussian Quadrature	683
E.6	Radau Quadrature	687
E.7	Lobatto Quadrature	690
E.8	Concluding Remarks	693
E.9	References	693
Nomenclature		694
Postface		698
Index		701