CONTENTS

Preface xvii

SECTION I PROCESS MODELING 1

1 Introduction 3

1.1 Motivation 3
1.2 Models 4
1.2.1 How Models Are Used 5
1.3 Systems 10
1.3.1 Simulation 10
1.3.2 Linear Systems Analysis 11
1.3.3 A Broader View of Analysis 11
1.4 Background of the Reader 12
1.5 How To Use This Textbook 12
1.5.1 Sections 12
1.5.2 Numerical Solutions 13
1.5.3 Motivating Examples and Modules 13
1.6 Courses Where This Textbook Can Be Used 13
Summary 14
Further Reading 14
Student Exercises 15

2 Process Modeling 16

2.1 Background 17
2.2 Balance Equations 17
2.2.1 Integral Balances 18
2.2.2 Instantaneous Balances 20
2.3 Material Balances 20
2.3.1 Simplifying Assumptions 25
2.4 Constitutive Relationships 27
2.4.1 Gas Law 27
2.4.2 Chemical Reactions 27
2.4.3 Equilibrium Relationships 28
2.4.4 Flow-through Valves 29
2.5 Material and Energy Balances 30
2.5.1 Review of Thermodynamics 31
2.6 Distributes Parameter Systems 34
2.7 Dimensionless Models 35
2.8 Explicit Solutions to Dynamic Models 36
2.9 General Form of Dynamic Models 37
2.9.1 State Variables 37
2.9.2 Input Variables
2.9.3 Parameters 38
2.9.4 Vector Notation 38
Summary 40
Further Reading 40
Student Exercises 41

SECTION II NUMERICAL TECHNIQUES 49

3 Algebraic Equations 51

3.1 Notations 51
3.2 General Form for a Linear System of Equations 51
3.3 Nonlinear Functions of a Single Variable 54
3.3.1 Convergence Tolerance 55
3.3.2 Direct Substitution 55
3.3.3 Interval Halving (Bisection) 58
3.3.4 False Position (Reguli Falsi) 60
3.3.5 Newton's Method (or Newton-Raphson) 60
3.4 MATLAB Routines for Solving Functions of a Single Variable 63
3.4.1 fzero 63
3.4.2 roots 64
3.5 Multivariable Systems 64
3.5.1 Newton's Method for Multivariable Problems 66
3.5.2 Quasi-Newton Methods 69

3.6 **MATLAB Routines for Systems of Nonlinear Algebraic Equations 70**
Summary 71
Further Reading 72
Student Exercises 73
Appendix 78

4 Numerical Integration 80

4.1 **Background 80**
4.2 **Euler Integration 81**
4.2.1 Explicit Euler 81
4.2.2 Implicit Euler 82
4.2.3 Numerical Stability of Explicit and Implicit Methods 83
4.3 **Runge-Kutta Integration 88**
4.3.1 Second Order Runge-Kutta 89
4.3.2 Fourth-Order Runge-Kutta 93
4.4 **MATLAB Integration Routines 94**
4.4.1 ode23 and ode45 95
Summary 97
Further Reading 97
Student Exercises 98

SECTION III LINEAR SYSTEMS ANALYSIS 103

5 Linearization of Nonlinear Models: The State-Space Formulation 105

5.1 **State Space Models 106**
5.5.1 General Form of State Space Models 108
5.2 **Linearization of Nonlinear Models 109**
5.2.1 Single Variable Example 109
5.5.2 One State Variable and One Input Variable 110
5.2.3 Linearization of Multistate Models 112
5.2.4 Generalization 114
5.3 **Interpretation of Linearization 117**
5.4 **Solution of the Zero-Input Form 119**
5.4.1 Effect of Initial Condition Direction (Use of Similarity Transform) 120
5.5 **Solution of the General State-Space Form 127**
5.6 **MATLAB Routines step and initial 127**
5.6.1 The MATLAB step Function 129
5.6.2 The MATLAB initial Function 129
Summary 130
Further Reading 131
Student Exercises 131

6 Solving Linear nth Order ODE Models 142

6.1 Background 143
6.2 Solving Homogeneous, Linear ODEs with Constant Coefficients 145
6.2.1 Distinct Eigenvalues 146
6.6.2 Repeated Eigenvalues 148
6.2.3 General Result for Complex Roots 152
6.3 Solving Nonhomogeneous, Linear ODEs with Constant Coefficients 152
6.4 Equations with Time-Varying Parameters 154
6.5 Routh Stability Criterion—Determining Stability Without Calculating Eigenvalues 157
6.5.1 Routh Array 157
Summary 160
Further Reading 161
Student Exercises 161

7 An Introduction to Laplace Transforms 168

7.1 Motivation 168
7.2 Definition of the Laplace Transform 169
7.3 Examples of Laplace Transforms 170
7.3.1 Exponential Function 170
7.3.3 Time-Delay (Dead Time) 172
7.3.4 Derivations 173
7.3.5 Integrals 173
7.3.6 Ramp Function 174
7.3.7 Pulse 174
7.3.8 Unit Impulse 176
7.3.9 Review 177
7.4 Final and Initial Value Theorems 177
7.5 Application Examples 178
7.5.1 Partial Fraction Expansion 179
7.6 Table of Laplace Transforms 185
Summary 187
Further Reading 187
Student Exercises 187

8 Transfer Function Analysis of First-Order Systems 190

8.1 Perspective 191
8.2 Responses of First-Order Systems 191
8.2.1 Step Inputs 193
8.2.2 Impulse Inputs 198
8.3 Examples of Self-Regulating Processes 200
8.4 Integrating Processes 206

8.5 **Lead-Lag Models 208**
8.5.1 Simulating Lead-Lag Transfer Functions 209
Summary 211
Student Exercises 211

9 **Transfer Function Analysis of Higher-Order Systems 215**

9.1 **Responses of Second-Order Systems 216**
9.1.1 Step Responses 217
9.1.2 Underdamped Step Response Characteristics 221
9.1.3 Impulse Responses 222
9.1.4 Response to Sine Inputs 224
9.2 **Second-Order Systems with Numerator Dynamics 226**
9.3 **The Effect of Pole-Zero Locations on System Step Responses 228**
9.4 **Padé Approximation for Deadtime 230**
9.5 **Converting the Transfer Function Model to State-Space Form 232**
9.6 **MATLAB Routines for Step and Impulse Response 234**
9.6.1 step 234
9.6.2 impulse 236
Summary 236
Student Exercises 237

10 **Matrix Transfer Functions 247**

10.1 **A Second-Order Example 248**
10.2 **The General Method 251**
10.3 **MATLAB Routine ss2tf 252**
10.3.1 Discussion of the Results from Example 10.2 255
Summary 257
Student Exercises 257

11 **Block Diagrams 261**

11.1 **Introduction to Block Diagrams 262**
11.2 **Block Diagrams of Systems in Series 262**
11.3 **Pole-Zero Cancellation 263**
11.4 **Systems in Series 267**
11.4.1 Simulating Systems in Series 267
11.5 **Blocks in Parallel 269**
11.5.1 Conditions for Inverse Response 271
11.6 **Feedback and Recycle Systems 273**
11.7 **Routh Stability Criterion Applied to Transfer Functions 276**
11.7.1 Routh Array 277
11.8 **SIMULINK 278**

Summary 279
Student Exercises 280

12 Linear Systems Summary 282

12.1 Background 283
12.2 Linear Boundary Value Problems 283
12.3 Review of Methods for Linear Initial Value Problems 287
12.3.1 Linearization 187
12.3.2 Direction Solution Techniques 288
12.3.3 Rewrite the State-Space Model as a Single nth Order Ordinary Differential Equation 289
12.3.4 Use Laplace Transforms Directly on the State-Space Model 290
12.4 Introduction to Discrete-Time Models 290
12.4.1 Discrete Transfer Function Models 291
12.5 Parameter Estimation of Discrete Linear Systems 295
Summary 297
References 297
Student Exercises 298

SECTION IV NONLINEAR SYSTEMS ANALYSIS 301

13 Phase-Plane Analysis 303

13.1 Background 304
13.2 Linear System Examples 304
13.3 Generalization of Phase-Plane Behavior 311
13.3.1 Slope Marks for Vector Fields 313
13.3.2 Additional Discussion 315
13.4 Nonlinear Systems 316
13.4.1 Limit Cycle Behavior 323
Summary 324
Further Reading 324
Student Exercises 324

14 Introduction Nonlinear Dynamics: A Case Study of the Quadratic Map 331

14.1 Background 332
14.2 A Simple Population Growth Model 332
14.3 A More Realistic Population Model 334
14.3.1 Transient Response Results for the Quadratic (Logistic) Map 335
14.4 Cobweb Diagrams 339
14.5 Bifurcation and Orbit Diagrams 342
14.5.1 Observations from the Orbit Diagram (Figure 14.14) 342

14.6 Stability of Fixed-Point Solutions 344
14.6.1 Application of the Stability Theorem to the Quadratic Map 344
14.6.2 Generalization of the Stability Results for the Quadratic Map 346
14.6.3 The Stability Theorem and Qualitative Behavior 346
14.7 Cascade of Period-Doublings 348
14.7.1 Period-2 348
14.7.2 Period-4 351
14.7.3 Period-n
14.7.4 Feigenbaum's Number 353
14.8 Further Comments on Chaotic Behavior 354
Summary 354
References and Further Reading 355
Student Exercises 356
Appendix: Matlab M-Files Used in This Module 358

15 Bifurcation Behavior of Single ODE Systems 360

15.1 Motivation 360
15.2 Illustration of Bifurcation Behavior 361
15.3 Types of Bifurcations 362
15.3.1 Dynamic Responses 365
Summary 376
References and Further Reading 376
Student Exercises 377
Appendix 379

16 Bifurcation Behavior of Two-State Systems 381

16.1 Background 381
16.2 Single-Dimensional Bifurcations in the Phase-Plane 382
16.3 Limit Cycle Behavior 384
16.4 The Hopf Bifurcation 388
16.4.1 Higher Order Systems (n > 2) 391
Summary 392
Further Reading 392
Student Exercises 392

17 Introduction to Chaos: The Lorenz Equations 395

17.1 Introduction 396
17.2 Background 396
17.3 The Lorenz Equations 397
17.3.1 Steady-State (Equilibrium) Solutions 398

17.4 Stability Analysis of the Lorenz Equations 399
17.4.1 Stability of the Trivial Solution 399
17.4.2 Stability of the Nontrivial Solutions 400
17.4.3 Summary of Stability Results 301
17.5 Numerical Study of the Lorenz Equations 402
17.5.1 Conditions for a Stable Trivial (No Flow) Solution 402
17.5.2 Stable Nontrivial Solutions 403
17.5.3 Chaotic Conditions 405
17.6 Chaos in Chemical Systems 407
17.7 Other Issues in Chaos 409
Summary 410
References and Further Reading 410
Student Exercises 411
Appendix 412

SECTION IV REVIEW AND LEARNING MODULES 413

Module 1 Introduction to MATLAB 415

M1.1 Background 416
M1.2 Using This Tutorial 416
M1.3 Entering Matrices 417
M1.4 The MATLAB Workspace 419
M1.5 Complex Variables 421
M1.6 Some MATLAB Operations 421
M1.7 Plotting 422
M1.8 More Matrix Stuff 426
M1.9 FOR Loops and IF-THEN Statements 427
M1.10 m-files 428
M1.11 Diary 430
M1.12 Toolboxes 430
M1.13 Limitations to Student MATLAB 431
M1.14 Contacting Mathworks 431
Student Exercises 432

Module 2 Review of Matrix Algebra 435

M2.1 Motivation and Notation 436
M2.2 Common Matrix Operations 436
M2.3 Square Matrices 440
M2.4 Other Matrix Operations 448
Summary 450
Student Exercises 450

Module 3 Linear Regression 452

M3.1 Motivation 452
M3.2 Least Squares Solution for a Line 454
M3.3 Solution for the Equation of a Line Using Matrix-Vector Notation 455
M3.4 Generalization of the Linear Regression Technique 456
M3.5 MATLAB Routines `polyfit` and `polyval` 458

Module 4 Introduction to SIMULINK 464

M4.1 Introduction 464
M4.2 Transfer Function-Based Simulation 466
M4.3 Printing SIMULINK Windows 469

Module 5 Stirred Tank Heaters 471

M5.1 Introduction 471
M5.2 Developing the Dynamic Model 472
M5.3 Steady-State Conditions 475
M5.4 State-Space Model 475
M5.5 Laplace Domain Model 477
M5.6 Step Responses: Linear versus Nonlinear Models 478
M5.7 Unforced System Responses: Perturbations in Initial Conditions 483

Module 6 Absorption 490

M6.1 Background 490
M6.2 The Dynamic Model 491
M6.3 Steady-State Analysis 495
M6.4 Step Responses 496
M6.5 Unforced Behavior 501

Module 7 Isothermal Continuous Stirred Tank Chemical Reactors 506

M7.1 Introduction 506
M7.2 First-Order Irreversible Reaction 507
M7.3 Van de Vusse Reaction 516

Module 8 Biochemical Reactors 529

M8.1 Background 529
M8.2 Modeling Equations 530
M8.3 Steady-State Solution 534
M8.4 Dynamic Behavior 535

M8.5 Linearization 536
M8.6 Phase-Plane Analysis 539
M8.7 Understanding Multiple Steady-States 540
M8.8 Bifurcation Behavior 549

Module 9 Diabatic Continuous Stirred Tank Reactors 559

M9.1 Background 560
M9.2 The Modeling Equations 561
M9.3 Steady-State Solution 563
M9.4 Dynamic Behavior 565
M9.5 Linearization of Dynamic Equations 567
M9.6 Phase-Plane Analysis 571
M9.7 Understanding Multiple Steady-State Behavior 572
M9.8 Further Complexities 580
M9.9 Dimensionless Model 584

Module 10 Ideal Binary Distillation 597

M10.1 Background 597
M10.2 Conceptual Description of Distillation 599
M10.3 Dynamic Material Balances 601
M10.4 Solving the Steady-State Equations 603
M10.5 Solving the Nonlinear Dynamic Equations 605
M10.6 State-Space Linear Distillation Models 606
M10.7 Multiplicity Behavior 608

Index 617