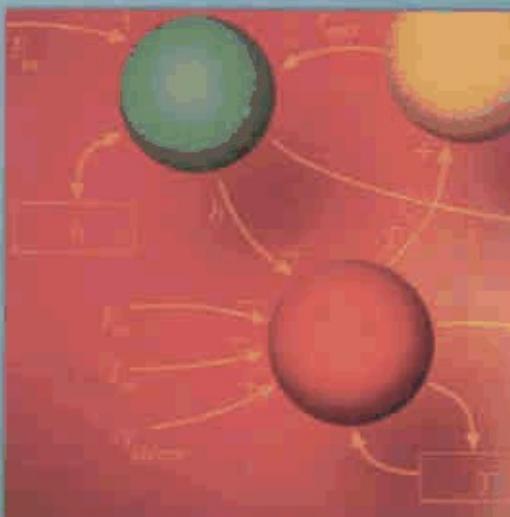
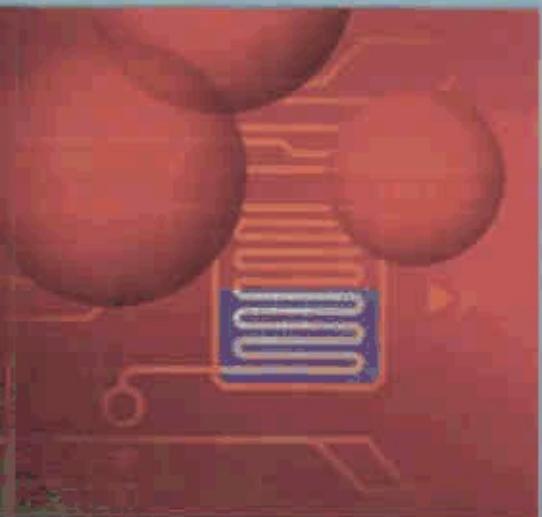


Brian Roffel and Ben Betlem



Process Dynamics and Control

Modeling for Control and Prediction

 WILEY



CONTENTS

Foreword	xi
Preface	xiii
Acknowledgement	xv
1 Introduction to Process Modeling.....	1
1.1 Application of Process Models.....	1
1.2 Dynamic Systems Modeling.....	2
1.3 Modeling Steps	5
1.4 Use of Diagrams	16
1.5 Types of Models	20
1.6 Continuous versus Discrete Models	23
References	23
2 Process Modeling Fundamentals	25
2.1 System States	25
2.2 Mass Relationship for Liquid and Gas	29
2.3 Energy Relationship	38
2.4 Composition Relationship	48
3 Extended Analysis of Modeling for Process Operation.....	57
3.1 Environmental Model	57
3.2 Procedure for the Development of an Environmental Model for Process Operation	58
3.3 Example: Mixer	68
3.4 Example: Evaporator with Variable Heat Exchanging Surface	69
4 Design for Process Modeling and Behavioral Models	71
4.1 Behavioral Model	71
4.2 Example: Mixer	77
5 Transformation Techniques.....	81
5.1 Introduction	81
5.2 Laplace Transform.....	81
5.3 Useful Properties of Laplace Transform: limit functions.....	83
5.4 Transfer Functions.....	84
5.5 Discrete Approximations	89
5.6 z -Transforms.....	90
References	95
6 Linearization of Model Equations	97
6.1 Introduction	97
6.2 Non-linear Process Models.....	97
6.3 Some General Linearization Rules.....	100
6.4 Linearization of Model of the Level Process	102
6.5 Linearization of the Evaporator model.....	103
6.6 Normalization of the Transfer Function	105
6.7 Linearization of the Chemical Reactor Model	105

7 Operating Points.....	109
7.1 Introduction	109
7.2 Stationary System and Operating Point.....	109
7.3 Flow Systems.....	110
7.4 Chemical System	111
7.5 Stability in the Operating Point	113
7.6 Operating Point Transition	116
8 Process Simulation	119
8.1 Using Matlab Simulink.....	119
8.2 Simulation of the Level Process	119
8.3 Simulation of the Chemical Reactor.....	124
References	126
9 Frequency Response Analysis	127
9.1 Introduction	127
9.2 Bode Diagrams	129
9.3 Bode Diagram of Simulink Models.....	135
References	137
10 General Process Behavior.....	139
10.1 Introduction	139
10.2 Accumulation Processes	140
10.3 Lumped Process with Non-interacting Balances.....	142
10.4 Lumped Process with Interacting Balances.....	144
10.5 Processes with Parallel Balances.....	148
10.6 Distributed Processes.....	151
10.7 Processes with Propagation Without Feedback.....	154
10.8 Processes with Propagation With Feedback.....	157
11 Analysis of a Mixing Process	161
11.1 The Process.....	161
11.2 Mixer with Self-adjusting Height.....	164
12 Dynamics of Chemical Stirred Tank Reactors.....	169
12.1 Introduction	169
12.2 Isothermal First-order Reaction.....	169
12.3 Equilibrium Reactions	172
12.4 Consecutive Reactions.....	175
12.5 Non-isothermal Reactions	178
13 Dynamic Analysis of Tubular Reactors	185
13.1 Introduction	185
13.2 First-order Reaction.....	186
13.3 Equilibrium Reaction	188
13.4 Consecutive Reactions.....	188
13.5 Tubular Reactor with Dispersion.....	188
13.6 Dynamics of Adiabatic Tubular Flow Reactors	192
References	194

14 Dynamic Analysis of Heat Exchangers	195
14.1 Introduction	195
14.2 Heat Transfer from a Heating Coil.....	195
14.3 Shell and Tube Heat Exchanger with Condensing Steam.....	198
14.4 Dynamics of a Counter-current Heat Exchanger	205
References	206
15 Dynamics of Evaporators and Separators	207
15.1 Introduction	207
15.2 Model Description	208
15.3 Linearization and Laplace Transformation	209
15.4 Derivation of the Normalized Transfer Function	210
15.5 Response Analysis.....	211
15.6 General Behavior.....	212
15.7 Example of Some Responses.....	212
15.8 Separation of Multi-phase Systems	213
15.9 Separator Model	214
15.10 Model Analysis.....	215
15.11 Derivation of the Transfer Function	217
16 Dynamic Modeling of Distillation Columns.....	219
16.1 Column Environmental Model	219
16.2 Assumptions and Simplifications.....	220
16.3 Column Behavioral Model	221
16.4 Component Balances and Equilibria	222
16.5 Energy Balances	225
16.6 Tray Hydraulics	228
16.7 Tray Pressure Drop.....	233
16.8 Column Dynamics	236
Notation	240
Greek Symbols	242
References	243
17 Dynamic Analysis of Fermentation Reactors	245
17.1 Introduction	245
17.2 Kinetic Equations	245
17.3 Reactor Models.....	247
17.4 Dynamics of the Fed-batch Reactor	248
17.5 Dynamics of Ideally Mixed Fermentation Reactor	252
17.6 Linearization of the Model for the Continuous Reactor	254
References	258
18 Physiological Modeling: Glucose-Insulin Dynamics and Cardiovascular Modeling.....	259
18.1 Introduction to Physiological Models	259
18.2 Modeling of Glucose and Insulin Levels	260
18.3 Steady-state Analysis.....	262
18.4 Dynamic Analysis	263
18.5 The Bergman Minimal Model	264
18.6 Introduction to Cardiovascular Modeling	264
18.7 Simple Model Using Aorta Compliance and Peripheral Resistance.....	265
18.8 Modeling Heart Rate Variability using a Baroreflex Model	268
References	271

19 Introduction to Black Box Modeling	273
19.1 Need for Different Model Types	273
19.2 Modeling steps.....	274
19.3 Data Preconditioning	275
19.4 Selection of Independent Model Variables	275
19.5 Model Order Selection	276
19.6 Model Linearity	277
19.7 Model Extrapolation.....	277
19.8 Model Evaluation	277
20 Basics of Linear Algebra	279
20.1 Introduction	279
20.2 Inner and Outer Product	280
20.3 Special Matrices and Vectors	281
20.4 Gauss–Jordan Elimination, Rank and Singularity.....	281
20.5 Determinant of a matrix.....	283
20.6 The Inverse of a Matrix	284
20.7 Inverse of a Singular Matrix.....	285
20.8 Generalized Least Squares	287
20.9 Eigen Values and Eigen Vectors	288
References	290
21 Data Conditioning	291
21.1 Examining the Data	291
21.2 Detecting and Removing Bad Data	292
21.3 Filling in Missing Data.....	295
21.4 Scaling of Variables	295
21.5 Identification of Time Lags	296
21.6 Smoothing and Filtering a Signal.....	297
21.7 Initial Model Structure	302
References	304
22 Principal Component Analysis.....	305
22.1 Introduction	305
22.2 PCA Decomposition.....	306
22.3 Explained Variance	308
22.4 PCA Graphical User Interface.....	309
22.5 Case Study: Demographic data	310
22.6 Case Study: Reactor Data	313
22.7 Modeling Statistics	314
References	316
23 Partial Least Squares	317
23.1 Problem Definition	317
23.2 The PLS Algorithm	318
23.3 Dealing with Non-linearities	319
23.4 Dynamic Extensions of PLS.....	320
23.5 Modeling Examples.....	321
References	325

24 Time-series Identification	327
24.1 Mechanistic Non-linear Models	327
24.2 Empirical (linear) Dynamic Models	327
24.3 The Least Squares Method	328
24.4 Cross-correlation and Autocorrelation	329
24.5 The Prediction Error Method.....	331
24.6 Identification Examples.....	332
24.7 Design of Plant Experiments	337
References	340
25 Discrete Linear and Non-linear State Space Modeling	341
25.1 Introduction	341
25.2 State Space Model Identification.....	342
25.3 Examples of State Space Model Identification	343
References	348
26 Model Reduction	349
26.1 Model Reduction in the Frequency Domain	349
26.2 Transfer Functions in the Frequency Domain.....	350
26.3 Example of Basic Frequency-weighted Model Reduction.....	351
26.4 Balancing of Gramians	353
26.5 Examples of Model State Reduction Techniques.....	356
References	360
27 Neural Networks.....	361
27.1 The Structure of an Artificial Neural Network	361
27.2 The Training of Artificial Neural Networks.....	363
27.3 The Standard Back Propagation Algorithm	364
27.4 Recurrent Neural Networks	367
27.5 Neural Network Applications and Issues	370
27.6 Examples of Models	372
References	379
28 Fuzzy Modeling	381
28.1 Mamdani Fuzzy Models.....	381
28.2 Takagi-Sugeno Fuzzy Models.....	382
28.3 Modeling Methodology	384
28.4 Example of Fuzzy Modeling	384
28.5 Data Clustering	386
28.6 Non-linear Process Modeling	391
References	397
29 Neuro Fuzzy Modeling.....	399
29.1 Introduction	399
29.2 Network Architecture	399
29.3 Calculation of Model Parameters	401
29.4 Identification Examples	403
References	410
30 Hybrid Models.....	413
30.1 Introduction	413
30.2 Methodology	414
30.3 Approaches for Different Process Types.....	424
30.4 Bioreactor Case Study	436
Literature	438

31 Introduction to Process Control and Instrumentation	439
31.1 Introduction	439
31.2 Process Control Goals	440
31.3 The Measuring Device	444
31.4 The Control Device	449
31.5 The Controller.....	451
31.6 Simulating the Controlled Process	452
References	453
32 Behaviour of Controlled Processes	455
32.1 Purpose of Control.....	455
32.2 Controller Equations.....	457
32.3 Frequency Response Analysis of the Process	458
32.4 Frequency Response of Controllers	460
32.5 Controller Tuning Guidelines.....	462
References	464
33 Design of Control Schemes.....	465
33.1 Procedure	465
33.2 Example: Desulphurization Process	472
33.3 Optimal Control	475
33.4 Extension of the Control Scheme	478
33.5 Final Considerations	485
34 Control of Distillation Columns.....	487
34.1 Control Scheme for a Distillation Column.....	487
34.2 Material and Energy Balance Control	495
Summary.....	500
References	501
Appendix 34.I Impact of Vapor Flow Variations on Liquid Holdup.....	501
Appendix 34.II Ratio Control for Liquid and Vapor Flow in the Column	502
35 Control of a Fluid Catalytic Cracker	503
35.1 Introduction	503
35.2 Initial Input–output Variable Selection	505
35.3 Extension of the Basic Control Scheme	509
35.4 Selection of the Final Control Scheme.....	510
References	514
Appendix A. Modeling an Extraction Process.....	515
A1: Problem Analysis.....	515
A2: Dynamic Process Model Development	517
A3: Dynamic Process Model Analysis	521
A4: Dynamic Process Simulation.....	524
A5: Process Control Simulation	530
Hints.....	534
Index	535