Contents

1 Introduction 1
1.1 Overview of the Main Topics 1
1.2 The Batch Reactor 2
1.2.1 The Case Study 3
1.3 Identification of Mathematical Models 4
1.4 Thermal Stability 4
1.5 Control of Batch Reactors 5
1.6 Fault Diagnosis for Chemical Batch Reactors 6
1.7 Applications to Non-ideal Reactors 7
1.8 Suggested Reading Paths 7

2 The Chemical Batch Reactor 9
2.1 Ideal Chemical Reactors 10
2.2 The Rate of Chemical Reactions 12
2.3 The Ideal Batch Reactor 15
2.3.1 Conservation of Mass 16
2.3.2 Conservation of Energy 20
2.4 Introducing the Case Study 22
2.4.1 Components 24
2.4.2 Reactions 25
2.5 A General Model for a Network of Nonchain Reactions 27
2.6 Measuring the Reactor Status 31
2.6.1 Measurements Quality 32
2.6.2 Online Measurements 32
2.6.3 Offline Measurements 35
2.7 Manipulating the Reactor Status 35
2.8 Conclusions 37
References 37

3 Identification of Kinetic Parameters 39
3.1 Bayesian Approach and Popper's Falsificationism 41
3.2 Experimental Data and Mathematical Models 43

3.3 Maximum Likelihood and Least Squares Criteria . . . 45
3.4 Optimization for Models Linear in the Parameters . . . 48
3.5 Optimization for Models Nonlinear in the Parameters . . . 50
3.5.1 Steepest Descent Algorithm . . . 50
3.5.2 Newton–Raphson Algorithm . . . 51
3.5.3 Levenberg–Marquardt Algorithm . . . 52
3.6 Implicit Models . . . 53
3.7 Statistical Analysis of the Results . . . 54
3.8 Case Study: Identification of Reduced Kinetic Models . . . 56
3.8.1 Reduced Models . . . 56
3.8.2 Generation of Data for Identification . . . 58
3.8.3 Estimating the Kinetic Parameters . . . 59
3.8.4 Estimating the Heats of Reaction . . . 61
3.8.5 Validation of the Reduced Models . . . 62
3.9 Conclusions . . . 65
References . . . 66

4 Thermal Stability . . . 69
4.1 Runaway in Chemical Batch Reactors . . . 70
4.2 Dimensionless Mathematical Model . . . 71
4.3 Adiabatic Reactor . . . 74
4.4 Isoperibolic Reactor . . . 75
4.4.1 The Semenov Theory . . . 76
4.4.2 Geometry-based Runaway Criteria . . . 79
4.4.3 Sensitivity-based Runaway Criteria . . . 82
4.5 Operation Limited by the Maximum Allowable Temperature . . . 84
4.6 Case Study: Runaway Boundaries . . . 85
4.7 Conclusions . . . 87
References . . . 87

5 Model-based Control . . . 89
5.1 Control Strategies for Batch Reactors . . . 91
5.2 PID Regulator . . . 92
5.3 Model Predictive Control . . . 93
5.4 Feedback Linearization . . . 95
5.4.1 Input–Output Linearization . . . 95
5.4.2 Generic Model Control . . . 96
5.5 State-Space Model for Control Design . . . 97
5.6 Estimation of the Heat Released by Reaction . . . 99
5.6.1 Model-Based Nonlinear Observer . . . 100
5.6.2 Model-Free Approaches . . . 102
5.7 Adaptive Two-Loop Control Scheme . . . 104
5.8 Case Study: Temperature Control . . . 108
5.8.1 Simulation Model . . . 109
5.8.2 Design of the Controller–Observer Scheme . . . 110
5.8.3 Discussion of Results . . . 111
5.8.4 Comparison with the PID Controller . . . 113

5.9 Conclusions . . . 116
References . . . 117

6 Fault Diagnosis . . . 121
6.1 Fault Diagnosis Strategies for Batch Reactors . . . 122
6.1.1 Model-Free Approaches . . . 123
6.1.2 Model-Based Approaches . . . 124
6.2 Basic Principles of Model-Based Fault Diagnosis . . . 125
6.2.1 Residual Generation . . . 127
6.2.2 Decision Making System and Fault Isolation . . . 128
6.3 Fault Diagnosis for Chemical Batch Reactors . . . 129
6.3.1 Fault Characterization . . . 129
6.3.2 Architecture of the Fault Diagnosis Scheme . . . 131
6.4 Sensor Fault Diagnosis . . . 133
6.4.1 Residuals Generation and Fault Isolation . . . 135
6.4.2 Determination of the Healthy Signal . . . 136
6.5 Actuator and Process Fault Diagnosis . . . 138
6.5.1 Fault Detection . . . 138
6.5.2 Fault Isolation and Identification . . . 140
6.6 Decoupling Sensor Faults from Process and Actuator Faults . . . 143
6.7 Case Study: Fault Diagnosis . . . 143
6.7.1 Simulation Results: Sensor Faults . . . 144
6.7.2 Simulation Results: Process and Actuator Faults . . . 148
6.7.3 Simulation Results: Sensor and Actuator Faults . . . 152
6.8 Conclusions . . . 155
References . . . 155

7 Applications to Nonideal Reactors . . . 159
7.1 Nonideal Batch Reactors . . . 160
7.2 Nonideal Mixing . . . 161
7.3 Multiphase Batch Reactors . . . 165
7.4 Scaling-up the Information . . . 166
7.4.1 Basic Ideas of Scale-up . . . 166
7.4.2 The Scale-up of Real Batch Reactors . . . 168
7.5 Suggestions and Conclusions . . . 169
References . . . 170

Appendix A Proofs . . . 171
A.1 Proof of Theorem 5.1 . . . 171
A.2 Proof of Theorem 5.2 . . . 173
A.3 Proof of Theorem 5.3 . . . 174
A.4 Proof of Theorem 5.4 . . . 175
A.5 Proof of Theorem 6.1 . . . 176
A.6 Proof of Theorem 6.2 . . . 178

Index . . . 181

Springer

http://www.springer.com/978-0-85729-194-3

Control and Monitoring of Chemical Batch Reactors
Caccavale, F.; Iamarino, M.; Pierri, F.; Tufano, V.
2011, XVII, 186 p., Hardcover
ISBN: 978-0-85729-194-3