Second Edition

Principles of Chemical Reactor Analysis and Design

New Tools for Industrial Chemical Reactor Operations

Uzi Mann

WILEY

CONTENTS

Preface xi

Notation xv

1 Overview of Chemical Reaction Engineering 1

1.1 Classification of Chemical Reactions, 2
1.2 Classification of Chemical Reactors, 3
1.3 Phenomena and Concepts, 8
1.3.1 Stoichiometry, 8
1.3.2 Chemical Kinetics, 9
1.3.3 Transport Effects, 9
1.3.4 Global Rate Expression, 14
1.3.5 Species Balance Equation and Reactor Design Equation, 14
1.3.6 Energy Balance Equation, 15
1.3.7 Momentum Balance Equation, 15
1.4 Common Practices, 15
1.4.1 Experimental Reactors, 16
1.4.2 Selection of Reactor Configuration, 16
1.4.3 Selection of Operating Conditions, 18
1.4.4 Operational Considerations, 18
1.4.5 Scaleup, 19
1.4.6 Diagnostic Methods, 20
1.5 Industrial Reactors, 20
1.6 Summary, 21
References, 22

2 Stoichiometry **25**

2.1 Four Contexts of Chemical Reaction, 25
2.2 Chemical Formulas and Stoichiometric Coefficients, 26
2.3 Extent of a Chemical Reaction, 28
2.4 Independent and Dependent Chemical Reactions, 39
2.5 Characterization of the Reactor Feed, 47
2.5.1 Limiting Reactant, 48
2.5.2 Excess Reactant, 49
2.6 Characterization of Reactor Performance, 54
2.6.1 Reactant Conversion, 54
2.6.2 Product Yield and Selectivity, 58
2.7 Dimensionless Extents, 64
2.8 Independent Species Composition Specifications, 68
2.9 Summary, 72
Problems, 72
Bibliography, 79

3 Chemical Kinetics **81**

3.1 Species Formation Rates, 81
3.2 Rates of Chemical Reactions, 82
3.3 Rate Expressions of Chemical Reactions, 86
3.4 Effects of Transport Phenomena, 91
3.5 Characteristic Reaction Time, 91
3.6 Summary, 97
Problems, 97
Bibliography, 99

4 Species Balances and Design Equations **101**

4.1 Macroscopic Species Balances—General Species-Based Design Equations, 102
4.2 Species-Based Design Equations of Ideal Reactors, 104
4.2.1 Ideal Batch Reactor, 104
4.2.2 Continuous Stirred-Tank Reactor (CSTR), 105
4.2.3 Plug-Flow Reactor (PFR), 106
4.3 Reaction-Based Design Equations, 107
4.3.1 Ideal Batch Reactor, 107
4.3.2 Plug-Flow Reactor, 109
4.3.3 Continuous Stirred-Tank Reactor (CSTR), 111
4.3.4 Formulation Procedure, 112
4.4 Dimensionless Design Equations and Operating Curves, 113

4.5 Summary, 125
Problems, 126
Bibliography, 129

5 Energy Balances **131**

5.1 Review of Thermodynamic Relations, 131
5.1.1 Heat of Reaction, 131
5.1.2 Effect of Temperature on Reaction Equilibrium Constant, 134
5.2 Energy Balances, 135
5.2.1 Batch Reactors, 136
5.2.2 Flow Reactors, 147
5.3 Summary, 156
Problems, 157
Bibliography, 158

6 Ideal Batch Reactor **159**

6.1 Design Equations and Auxiliary Relations, 160
6.2 Isothermal Operations with Single Reactions, 166
6.2.1 Constant-Volume Reactors, 167
6.2.2 Gaseous, Variable-Volume Batch Reactors, 181
6.2.3 Determination of the Reaction Rate Expression, 189
6.3 Isothermal Operations with Multiple Reactions, 198
6.4 Nonisothermal Operations, 216
6.5 Summary, 230
Problems, 231
Bibliography, 238

7 Plug-Flow Reactor **239**

7.1 Design Equations and Auxiliary Relations, 240
7.2 Isothermal Operations with Single Reactions, 245
7.2.1 Design, 246
7.2.2 Determination of Reaction Rate Expression, 261
7.3 Isothermal Operations with Multiple Reactions, 265
7.4 Nonisothermal Operations, 281
7.5 Effects of Pressure Drop, 296
7.6 Summary, 308
Problems, 309

8 Continuous Stirred-Tank Reactor 317

8.1 Design Equations and Auxiliary Relations, 318
8.2 Isothermal Operations with Single Reactions, 322
8.2.1 Design of a Single CSTR, 324
8.2.2 Determination of the Reaction Rate Expression, 333
8.2.3 Cascade of CSTRs Connected in Series, 336
8.3 Isothermal Operations with Multiple Reactions, 341
8.4 Nonisothermal Operations, 358
8.5 Summary, 370
Problems, 370

9 Other Reactor Configurations 377

9.1 Semibatch Reactors, 377
9.2 Plug-Flow Reactor with Distributed Feed, 400
9.3 Distillation Reactor, 416
9.4 Recycle Reactor, 425
9.5 Summary, 435
Problems, 435

10 Economic-Based Optimization 441

10.1 Economic-Based Performance Objective Functions, 442
10.2 Batch and Semibatch Reactors, 448
10.3 Flow Reactors, 450
10.4 Summary, 453
Problems, 453
Bibliography, 454

Appendix A Summary of Key Relationships 455

Appendix B Microscopic Species Balances—Species Continuity Equations 465

Appendix C Summary of Numerical Differentiation and Integration 469

Index 471