660.2832man2nded

CONTENTS

Preface

Notation

1

1 Overview of Chemical Reaction Engineering

- 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

1.0

- 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

viii CONTENTS

Stoichiometry 2

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

Chemical Kinetics 3

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

Species Balances and Design Equations 4

Macroscopic Species Balances—General Species-Based 4.1 Design Equations, 102

Species-Based Design Equations of Ideal Reactors, 104 4.2

- 4.2.1 Ideal Batch Reactor, 104
- 4.2.2 Continuous Stirred-Tank Reactor (CSTR), 105
- 4.2.3 Plug-Flow Reactor (PFR), 106
- Reaction-Based Design Equations, 107 4.3
 - 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
- **Dimensionless Design Equations and** 4.4 Operating Curves, 113



4.5 Summary, 125Problems, 126Bibliography, 129

5 Energy Balances

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

- 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

159

131

- 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

- 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

239



x CONTENTS

317

8 Continuous Stirred-Tank Reactor

- 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

- 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

377

	10 Ec	Economic-Based Optimization		
	10.		conomic-Based Performance Objective Functions, 442	
			tch and Semibatch Reactors, 448	
10.3 Flow Reactors, 450 10.4 Summary, 453				
Problem				
		Bibliography, 454		
	Append	lix A	Summary of Key Relationships	455
	Append	lix B	Microscopic Species Balances—Species Continuity Equations	465
	Append	lix C	Summary of Numerical Differentiation and Integration	469
	Index			471