

Contents

Preface	xv
Acknowledgments	xxi
Notation	xxxii
1 Multiphase Reactors: Types, Characteristics, and Uses	
A. Gianetto	1
1.1 Introduction	1
1.2 Reactors with Moving Solids	2
1.2.1 <i>Stirred Slurry Reactors</i>	2
1.2.2 <i>Bubbling Slurry Column</i>	2
1.2.3 <i>Fluidized Slurry Reactor</i>	3
1.2.4 <i>Cocurrent Upflow Reactor with Fluidized Solids</i>	4
1.3 Reactors with Fixed Beds of Solids	4
1.3.1 <i>Submerged Fixed Bed Reactor with Gas Bubbling</i>	4
1.3.2 <i>Trickle Bed Reactor</i>	5
1.4 Criteria for Choosing Specific Types of Multiphase Reactors	6
1.5 Industrial Applications of Multiphase Reactors	10
1.6 Fundamental Phenomena in Multiphase Reactors	14
1.7 Design Criteria for Mechanically Stirred Reactors	16
1.8 Design Criteria for Fixed-Bed Reactors	19
Notation	27
References	28
2 Mass Transfer Coupled with Chemical Reaction	
J.-C. Charpentier	32
2.1 Introduction	32
2.2 Analysis of the Gas-Liquid Reaction System	33
2.2.1 <i>Reactor Equations</i>	34
2.2.2 <i>Interfacial Condition</i>	38
2.2.3 <i>Use of the Hatta Number</i>	40
2.3 Mass Transfer in Gas-Liquid Reactors	44
2.3.1 <i>Physical Absorption</i>	45
2.3.2 <i>Mass Transfer with Chemical Reaction</i>	48
2.3.4 <i>Desorption</i>	65
2.3.5 <i>Thermal Effects in Gas Absorption</i>	69
2.3.6 <i>Simultaneous Absorption of Two Reacting Gases</i>	73
Notation	76
References	79

3	Solubility and Diffusivity of Gases in Liquids		
	<i>J.-C. Charpentier</i>		81
3.1	Introduction		81
3.2	Solubility of Gases in Liquids		81
	3.2.1 <i>Solubility in Nonelectrolytes</i>		82
	3.2.2 <i>Solubility in Electrolytes</i>		89
3.3	Diffusivity in Liquids		91
	3.3.1 <i>Diffusivity in Nonelectrolytes</i>		91
	3.3.2 <i>Diffusivity in Electrolytes</i>		96
	Notation		98
	References		100
4	Measurement of Gas-Liquid Parameters	<i>J.-C. Charpentier</i>	104
4.1	Physical Techniques		104
	4.1.1 <i>Gas Holdup</i>		104
	4.1.2 <i>Bubble Size</i>		106
	4.1.3 <i>Interfacial Area</i>		106
	4.1.4 <i>Discussion of Physical Methods</i>		107
4.2	Chemical Techniques		109
	4.2.1 <i>Determination of the Volumetric Mass Transfer Coefficient</i>		109
	4.2.2 <i>Determination of the Volumetric Coefficient, using a Slow Irreversible Reaction</i>		109
	4.2.3 <i>Determination of the Volumetric Coefficient using an Instantaneous Irreversible Chemical Reaction</i>		111
	4.2.4 <i>Determination of the Gas-Liquid Interfacial Area</i>		112
	4.2.5 <i>Determination of the Gas Side Volumetric Coefficient</i>		114
	4.2.6 <i>Simultaneous Measurement of Volumetric Mass Transfer Coefficients and Interfacial Area</i>		116
	4.2.7 <i>Laboratory Equipment for Determination of the Physicochemical Parameters by Chemical Methods</i>		118
	4.2.8 <i>Application to the Kinetics of the Oxidation of Aqueous Sodium Sulphite Solutions</i>		125
	4.2.9 <i>Limits of the Chemical Technique Introduced by Inhibited Bubble Coalescence</i>		133
	4.2.10 <i>Application of the Chemical Technique to Organic Liquid Phases</i>		136
4.3	Mass Transfer Data for Chemical and Purely Physical Processes		138
	Notation		144
	References		149

5	Simulation of Industrial and Pilot Scale Gas-Liquid Absorbers by Laboratory Scale Models	<i>J.-C. Charpentier</i>	152
5.1	Criteria for Simulation		152
5.2	Practical Selection of a Laboratory Model to Simulate an Industrial Absorber		154
5.2.1	<i>Absorption and Reaction in the Liquid Film with a Pure Gas</i>		154
5.2.2	<i>Absorption and Reaction in the Liquid Film with a Dilute Gas Solute</i>		156
5.2.3	<i>Absorption and Complete Reaction with a Dilute Gas Solute</i>		157
5.3	Practical Examples of Simulation		157
5.3.1	<i>Simulation of a Point in a Packed Column by a Stirred Cell</i>		157
5.3.2	<i>Simulation of a Packed Column Absorber by a String of Spheres (Uses of an Integral Model)</i>		159
5.3.3	<i>Simulation of a Pilot Scale Venturi Jet Scrubber by a Laminar Jet</i>		162
	Notation		169
	References		172
6	Reaction within Porous Catalysts—Effectiveness Factors		
	<i>P. L. Silveston</i>		173
6.1	Introduction		173
6.2	Consequence of Transport Resistance in Porous Solids		174
6.2.1	<i>Model for Concentration Change</i>		174
6.2.2	<i>Formulation of Mathematical Relationships</i>		176
6.2.3	<i>Concept of an Effectiveness Factor</i>		180
6.2.4	<i>Effectiveness Factors for Non-First-Order Reactions</i>		185
6.2.5	<i>Measured Effectiveness Factors</i>		192
6.2.6	<i>Falsification of Kinetic Parameters</i>		192
6.2.7	<i>Effects of Internal Diffusion on Selectivity</i>		197
6.2.8	<i>Tests for the Significance of Internal Diffusion</i>		204
6.2.9	<i>Non-Isothermal Systems</i>		205
6.2.10	<i>Volume Change Reactions</i>		207
6.3	Overall Effectiveness Factors and Observable Thiele Moduli		207
6.3.1	<i>Overall Effectiveness Factors</i>		207
6.3.2	<i>Extension to Three-Phase Systems</i>		209
6.3.3	<i>Contacting Effectiveness</i>		211
6.3.4	<i>Influence of Wetting</i>		211
6.3.5	<i>Observable Thiele Modulus</i>		212

6.4	Effectiveness Factors with Nonsymmetrical External Concentrations	215
6.5	Effectiveness Factors with Gas-filled or Partially Filled Pores	216
6.6	Kinetic Measurement in Multiphase Systems	217
6.6.1	<i>Requirements for Kinetics Studies in Slurry Reactors</i>	217
6.6.2	<i>Tests for Significance of Transport in Slurry Reactors</i>	218
6.6.3	<i>Interpretation of Data in the Presence of Diffusional Interference</i>	218
	Notation	219
	References	224
7	Effective Diffusivity and Structure of Porous Catalysts	
	<i>P. L. Silveston</i>	228
7.1	Experimental Measurements of Effective Diffusivity	228
7.1.1	<i>Steady State Transport</i>	229
7.1.2	<i>Pulse Method</i>	231
7.2	Structure of Porous Solids	236
7.3	Pore Structure Models and Effective Diffusivity Estimates	240
7.3.1	<i>Pore Bundle Models</i>	240
7.3.2	<i>Grain Models</i>	243
7.3.3	<i>Grain Models with Porous Particles</i>	244
7.3.4	<i>Shape Change and Branching Models</i>	246
7.3.5	<i>Bidispersed Pore-size Distributions</i>	247
7.3.6	<i>Random Pore Model</i>	248
7.4	Experimental Tortuosity	250
	Notation	252
	References	255
8	Hydrodynamics and Hydrodynamic Models of Fixed Bed Reactors	
	<i>H. Hofmann</i>	257
8.1	Introduction	257
8.2	Hydrodynamic Characteristics of Three Phase Catalytic Fixed Bed Reactors	258
8.2.1	<i>Mode of Operation and Flow Regimes</i>	258
8.2.2	<i>Pressure Drop</i>	260
8.2.3	<i>Degree of Wetting of the Catalyst and Hydrodynamics</i>	263
8.2.4	<i>Holdup of the Phases and Dispersion as Characteristics of Hydrodynamics</i>	266

8.2.5	<i>Hydrodynamic Effects on Mass Transfer</i>	269
8.3	Hydrodynamic Models and Their Application	273
8.3.1	<i>Limitations Imposed by Hydrodynamics</i>	273
8.3.2	<i>Use of Models</i>	273
8.3.3	<i>Continuum Models</i>	274
8.3.4	<i>Other Models</i>	281
8.4	Summary	281
	Notation	282
	References	285
9	Mass Transfer in Fixed Bed Reactors <i>J.-C. Charpentier</i>	289
9.1	Countercurrent Packed Columns	289
9.2	Countercurrent Packed Bubble Columns	297
9.3	Cocurrent Packed Columns	297
9.3.1	<i>Hydrodynamics</i>	299
9.3.2	<i>Gas-Liquid Mass Transfer</i>	307
9.3.3	<i>Liquid-Solid Mass Transfer</i>	329
	Notation	342
	References	346
10	Liquid-Solid Contacting Effectiveness in Trickle Bed Reactors <i>J. M. Smith</i>	350
10.1	Introduction	350
10.2	Physical System	350
10.3	Effectiveness Factors with Unsymmetrical Boundary Conditions	352
10.3.1	<i>Particle Effectiveness Factors, Slab Geometry ($f = 0.5$)</i>	352
10.3.2	<i>Overall Effectiveness Factor, Slab Geometry ($f = 0.5$)</i>	355
10.4	Weighting Factor Models for Overall Effectiveness Factors in Trickle Beds	357
10.4.1	<i>Slab Geometry</i>	357
10.4.2	<i>Spherical Geometry</i>	359
10.4.3	<i>Cubical Model</i>	361
10.5	Comparison of Effectiveness Factor Models	362
10.6	Prediction of Reaction Rates with Partial Wetting	363
10.7	Estimation of Wetting Efficiencies	368
10.8	Criterion for the Importance of Partial Wetting	369
10.9	Rivulet Distribution	371
	Notation	371
	References	373

11	Heat Transfer in Fixed Bed Three Phase Reactors		
	<i>G. Baldi</i>		375
11.1	Introduction		375
11.2	Heat Transport Processes		375
	11.2.1 <i>Intraparticle Heat Transport</i>		376
	11.2.2 <i>Interphase Heat Transport</i>		380
	11.2.3 <i>Interparticle Heat Transfer</i>		383
11.3	Temperature Control in Three Phase Reactors		387
	11.3.1 <i>Thermal Instability</i>		387
	11.3.2 <i>Temperature Control</i>		391
	Notation		392
	References		395
12	Scale Up Strategies for Trickle Bed Reactors	<i>A. Gianetto</i>	398
12.1	Introduction		398
12.2	Experimental Reactors		398
	12.2.1 <i>Multisphere Reactor</i>		398
	12.2.2 <i>Recycle Reactors</i>		399
	12.2.3 <i>Differential Reactors</i>		401
12.3	Use of Models		402
12.4	Phenomenological Considerations in Model Development		406
	12.4.1 <i>End Effects</i>		407
	12.4.2 <i>Axial Dispersion</i>		407
	12.4.3 <i>Homogeneous Reactions</i>		408
	12.4.4 <i>Interphase Mass Transfer</i>		409
	12.4.5 <i>Incomplete Wetting of the Catalyst</i>		413
	12.4.6 <i>Thermal Gradients</i>		421
12.5	Recommendations		425
	Notation		425
	References		428
13	Hydrodynamics and Mass Transfer in Bubble Columns		
	<i>H. Hofmann</i>		432
13.1	Industrial Application and Technological Aspects		432
13.2	Hydrodynamics		433
	13.2.1 <i>Flow Regimes</i>		433
	13.2.2 <i>Pressure Drop</i>		433
	13.2.3 <i>Hold Up and Dispersion</i>		439
	13.2.4 <i>Bubble Size and Effective Bubble Rise Velocity</i>		446
	13.2.5 <i>Interfacial Area</i>		447
13.3	Mass and Heat Transfer		
	13.3.1 <i>Liquid Side Volumetric Mass Transfer Coefficients</i>		449

13.3.2	<i>Liquid-Solid Mass Transfer Coefficients</i>	450
13.3.3	<i>Fluid-Solid Heat Transfer Coefficients</i>	453
13.3.4	<i>Effective Thermal Conductivity and Wall Heat Transfer Coefficients</i>	453
13.4	Reactor Models	454
13.4.1	<i>Continuum Models</i>	454
13.4.2	<i>Staged Models</i>	456
13.4.3	<i>Zone Models</i>	456
13.5	Summary	457
	Notation	461
	References	
14	Hydrodynamics and Gas-Liquid Mass Transfer in Stirred Slurry Reactors <i>G. Baldi</i>	465
14.1	Introduction	465
14.2	Hydrodynamics	465
14.2.1	<i>Geometrical Configurations</i>	466
14.2.2	<i>Hydrodynamic Regimes</i>	468
14.2.3	<i>Power Dissipated</i>	475
14.2.4	<i>Gas Holdup</i>	479
14.2.5	<i>Solid Suspension</i>	485
14.3	Mass Transfer	489
14.3.1	<i>Methods for Measuring Mass Transfer Coefficients</i>	491
14.3.2	<i>Mass Transfer Coefficients and Interfacial Area</i>	495
14.4	Reactor Models	502
	Notation	503
	References	505
15	Models for Slurry Reactors <i>J. M. Smith</i>	511
15.1	Introduction	511
15.2	Mixing Characteristics	511
15.2.1	<i>Mixing in the Liquid Phase</i>	511
15.2.2	<i>Mixing in the Gas Phase</i>	512
15.3	Slurry Reactor Models	516
15.3.1	<i>Global Reaction Rate</i>	516
15.3.2	<i>Reactor Mass Conservation Equations</i>	522
15.3.3	<i>Adequacy of Proposed Models</i>	528
	Notation	529
	References	531

16 Applications to Hydrotreating and Other Hydrogenation Processes	<i>A. Gianetto and P. L. Silveston</i>	533
16.1	Introduction	533
16.2	Hydroprocessing of Petroleum Crude Fractions and Other Refinery Streams	533
16.2.1	<i>Hydrodesulfurization</i>	534
16.2.2	<i>Hydrocracking</i>	549
16.3	Hydrogenation of Chemical Compounds	553
16.3.1	<i>Hydrogenation of Benzene to Cyclohexane</i>	553
16.3.2	<i>Hydrogenation of Benzoic to Cyclohexane Carboxylic Acid</i>	555
16.3.3	<i>Hydrogenation of Adiponitrile to Hexamethylene Diamine</i>	556
16.3.4	<i>Hydrogenation of Caprolactone to 1,6 Hexanediol</i>	557
16.3.5	<i>Hydrogenolysis of Long-Chain Esters to Produce Higher Alcohols</i>	557
16.3.6	<i>Hydrogenation of Carbohydrates</i>	559
	Notation	561
	References	562
17 Application to Coal Liquefaction	<i>P. L. Silveston</i>	564
17.1	Introduction	564
17.2	Overview of Major Liquefaction Processes	565
17.2.1	<i>Solvent Refining</i>	565
17.2.2	<i>Direct Hydrogenation</i>	570
17.3	Nature of Coal	571
17.3.1	<i>Mineralogical Description</i>	573
17.3.2	<i>Chemical Characterization</i>	575
17.3.3	<i>Physical Character</i>	580
17.4	Dissolution and Hydrogenation Mechanism	581
17.5	Liquefaction Kinetics	585
17.6	Reactor Design	591
17.6.1	<i>Preheater Design</i>	591
17.6.2	<i>Hydrogenation Reactor Design</i>	594
17.6.3	<i>Solvent Hydrogenator Design</i>	598
	Notation	598
	References	599
18 Design of Multiphase Reactors for Biological Processes		
	<i>Murray Moo-Young</i>	601
18.1	Introduction	601

18.1.1	<i>Reactor Types and Transfer Implications</i>	601
18.1.2	<i>Systems and Operating Constraints</i>	602
18.2	Intrinsic Bioreaction Kinetics	606
18.3	Physical Pathways	607
18.3.1	<i>Rate Controlling Steps</i>	607
18.3.2	<i>Definition of the Transfer Coefficient</i>	608
18.3.3	<i>Effect of Diffusion</i>	610
18.3.4	<i>Effect of Interfacial Phenomena</i>	611
18.4	Interparticle Transfer Rates	612
18.4.1	<i>Basic Parameters</i>	612
18.4.2	<i>Particles in Stagnant Environments</i>	613
18.4.3	<i>Particles with Rigid Surfaces in Moving Fluids</i>	614
18.4.4	<i>Particles with Mobile Surfaces in Moving Fluids</i>	616
18.4.5	<i>Interacting Particles</i>	617
18.4.6	<i>Non-Newtonian Flow Effects</i>	617
18.4.7	<i>Effect of Bulk Mixing Patterns</i>	618
18.5	Intraparticle Bioreaction Rates	618
18.5.1	<i>General Concepts</i>	618
18.5.2	<i>Oxygen Transfer in Mold Pellets</i>	619
18.5.3	<i>Immobilized Enzymes</i>	620
18.5.4	<i>Enzymatic Degradation of Insoluble Substrates</i>	621
18.6	Physical Properties of Bioreactor Media	621
18.6.1	<i>Rheological Properties</i>	621
18.6.2	<i>Basic Dispersion Properties</i>	623
18.6.3	<i>Gas Flow Effect on Bubble Swarms</i>	624
18.7	Bioreactor Equipment Performance	625
18.7.1	<i>Bubble Columns</i>	625
18.7.2	<i>Systems with Stationary Internals</i>	626
18.7.3	<i>Special Tubular Devices</i>	627
18.7.4	<i>Mechanically Stirred Tanks</i>	629
18.8	Basic Hardware and Efficiencies	633
18.9	Power and Scale up	637
18.9.1	<i>General Concepts</i>	637
18.9.2	<i>Power in Ungassed Systems</i>	637
18.9.3	<i>Power in Gassed Systems</i>	639
18.9.4	<i>Scale up on a Flow System</i>	641
	Acknowledgments	641
	Notation	642
	References	645
	About the Authors	649
	Subject Index	653