PREFACE		XV
ABOUT THE AU	THOR	xxix
CHAPTER 1 M	OLE BALANCES	1
1.1	The Rate of Reaction, $-r_A$ 4	
1.2	The General Mole Balance Equation 8	
1.3	Batch Reactors (BRs) 10	
1.4	Continuous-Flow Reactors 12 1.4.1 Continuous-Stirred Tank Reactor (CSTR) 12 1.4.2 Tubular Reactor 14 1.4.3 Packed-Bed Reactor (PBR) 18	
1.5	Industrial Reactors 22	
CHAPTER 2 C	ONVERSION AND REACTOR SIZING Definition of Conversion 34	33
2.2	Batch Reactor Design Equations 34	
2.3	Design Equations for Flow Reactors 37 2.3.1 CSTR (Also Known as a Backmix Reactor or a Vat) 38 2.3.2 Tubular Flow Reactor (PFR) 38 2.3.3 Packed-Bed Reactor (PBR) 39	
2.4	Sizing Continuous-Flow Reactors 40	
2.5	Reactors in Series 49 2.5.1 CSTRs in Series 50 2.5.2 PFRs in Series 54	

Viii Contents

	 2.5.3 Combinations of CSTRs and PFRs in Series 55 2.5.4 Comparing the CSTR and PFR Reactor Volumes and Reactor Sequencing 59
2.6	Some Further Definitions 60 2.6.1 Space Time 60 2.6.2 Space Velocity 62
CHAPTER 3 R	ATE LAWS
3.1	Basic Definitions 74 3.1.1 Relative Rates of Reaction 74
3.2	The Reaction Order and the Rate Law 76 3.2.1 Power Law Models and Elementary Rate Laws 76 3.2.2 Nonelementary Rate Laws 80 3.2.3 Reversible Reactions 83
3.3	The Reaction Rate Constant 86
3.4	Present Status of Our Approach to Reactor Sizing and Design 93
4.1	Batch Systems 107 4.1.1 Equations for Batch Concentrations 109 Flow Systems 113 4.2.1 Equations for Concentrations in Flow Systems 114 4.2.2 Liquid-Phase Concentrations 114 4.2.3 Gas Phase Concentrations 115
CHAPTER 5 15	SOTHERMAL REACTOR DESIGN: CONVERSION Design Structure for Isothermal Reactors 140
5.2	Batch Reactors (BRs) 144 5.2.1 Batch Reaction Times 144
5.3	Continuous Stirred Tank Reactors (CSTRs) 152 5.3.1 A Single CSTR 152 5.3.2 CSTRs in Series 155
5.4	Tubular Reactors 162
5.5	Pressure Drop in Reactors 169 5.5.1 Pressure Drop and the Rate Law 169 5.5.2 Flow Through a Packed Bed 170 5.5.3 Pressure Drop in Pipes 174 5.5.4 Analytical Solution for Reaction with Pressure Drop 177
5.6	Synthesizing the Design of a Chemical Plant 188

CHAPTER 6 IS	SOTHERMAL REACTOR DESIGN: MOLAR FLOW RATES	207
6.1	The Molar Flow Rate Balance Algorithm 208	
6.2	Mole Balances on CSTRs, PFRs, PBRs, and Batch Reactors 6.2.1 Liquid Phase 208 6.2.2 Gas Phase 210	
6.3	Applications of the Molar Flow Rate Algorithm to Microreactors 212	
6.4	Membrane Reactors 217	
6.5	Unsteady-State Operation of Stirred Reactors 225	
6.6	Semibatch Reactors 226 6.6.1 Motivation for Using a Semibatch Reactor 226 6.6.2 Semibatch Reactor Mole Balances 227	
CHAPTER 7 C	OLLECTION AND ANALYSIS OF RATE DATA	245
7.1	The Algorithm for Data Analysis 246	
7.2	Determining the Reaction Order for Each of Two Reactants Using the Method of Excess 248	
7.3	Integral Method 249	
7.4	Differential Method of Analysis 253 7.4.1 Graphical Differentiation Method 254 7.4.2 Finding the Rate Law Parameters 254	
7.5	Nonlinear Regression 259	
7.6	Reaction Rate Data from Differential Reactors 264	
7.7	Experimental Planning 271	
CHAPTER 8 M	IULTIPLE REACTIONS	283
8.1	Definitions 283 8.1.1 Types of Reactions 283 8.1.2 Selectivity 285 8.1.3 Yield 286	
8.2	Algorithm for Multiple Reactions 286 8.2.1 Modifications to the Chapter 6 CRE Algorithm for Multiple Reactions 288	
8.3	Parallel Reactions 289 8.3.1 Selectivity 289 8.3.2 Maximizing the Desired Product for One Reactant 289 8.3.3 Reactor Selection and Operating Conditions 295	
8.4	Reactions in Series 298	
8.5	Complex Reactions 308 8.5.1 Complex Reactions in a PBR 308 8.5.2 Multiple Reactions in a CSTR 311	

X Contents

8.6	Membrane Reactors to Improve Selectivity in Multiple Reactions 316	
8.7	Sorting It All Out 321	
8.8	The Fun Part 321	
	EACTION MECHANISMS, PATHWAYS, BIOREACTIONS, ND BIOREACTORS	339
9.1	Active Intermediates and Nonelementary Rate Laws 9.1.1 Pseudo-Steady-State Hypothesis (PSSH) 341 9.1.2 Searching for a Mechanism 345 9.1.3 Chain Reactions 348	
9.2	Enzymatic Reaction Fundamentals 349 9.2.1 Enzyme–Substrate Complex 350 9.2.2 Mechanisms 352 9.2.3 Michaelis–Menten Equation 354 9.2.4 Batch Reactor Calculations for Enzyme Reactions 359	
9.3	Inhibition of Enzyme Reactions 364 9.3.1 Competitive Inhibition 364 9.3.2 Uncompetitive Inhibition 367 9.3.3 Noncompetitive Inhibition (Mixed Inhibition) 368 9.3.4 Substrate Inhibition 370	
9.4	Bioreactors and Biosynthesis 371 9.4.1 Cell Growth 375 9.4.2 Rate Laws 376 9.4.3 Stoichiometry 379 9.4.4 Mass Balances 383 9.4.5 Chemostats 387 9.4.6 CSTR Bioreactor Operation 388 9.4.7 Wash-Out 389	
CHAPTER 10	CATALYSIS AND CATALYTIC REACTORS	409
10.1	Catalysts 409 10.1.1 Definitions 410 10.1.2 Catalyst Properties 411 10.1.3 Catalytic Gas-Solid Interactions 413 10.1.4 Classification of Catalysts 414	
10.2	Steps in a Catalytic Reaction 415 10.2.1 Step 1 Overview: Diffusion from the Bulk to the External Surface of the Catalyst 418 10.2.2 Step 2 Overview: Internal Diffusion 419 10.2.3 Adsorption Isotherms 420 10.2.4 Surface Reaction 426	

	10.2.5 Desorption 428 10.2.6 The Rate-Limiting Step 428	
10.3	Synthesizing a Rate Law, Mechanism, and Rate-Limiting Step 10.3.1 Is the Adsorption of Cumene Rate-Limiting? 434 10.3.2 Is the Surface Reaction Rate-Limiting? 437 10.3.3 Is the Desorption of Benzene Rate-Limiting? 439 10.3.4 Summary of the Cumene Decomposition 440 10.3.5 Reforming Catalysts 441 10.3.6 Rate Laws Derived from the Pseudo-Steady-State Hypothesis (PSSH) 445 10.3.7 Temperature Dependence of the Rate Law 446	
10.4	Heterogeneous Data Analysis for Reactor Design 446 10.4.1 Deducing a Rate Law from the Experimental Data 448 10.4.2 Finding a Mechanism Consistent with Experimental Observations 449 10.4.3 Evaluation of the Rate Law Parameters 450 10.4.4 Reactor Design 453	
10.5	Reaction Engineering in Microelectronic Fabrication 10.5.1 Overview 456 10.5.2 Chemical Vapor Deposition 458	
10.6	Model Discrimination 461	
S	IONISOTHERMAL REACTOR DESIGN–THE STEADY TATE ENERGY BALANCE AND ADIABATIC PFR PPLICATIONS	477
11.1	Rationale 478	
11.2	The Energy Balance 479 11.2.1 First Law of Thermodynamics 479 11.2.2 Evaluating the Work Term 480 11.2.3 Overview of Energy Balances 482	
11.3	The User Friendly Energy Balance Equations 486 11.3.1 Dissecting the Steady-State Molar Flow Rates to Obtain the Heat of Reaction 486 11.3.2 Dissecting the Enthalpies 488 11.3.3 Relating $\Delta H_{\rm Rx}(T)$, $\Delta H_{\rm Rx}^{\circ}(T_{\rm R})$, and $\Delta C_{\rm P}$ 489	
11.4	Adiabatic Operation 492 11.4.1 Adiabatic Energy Balance 492 11.4.2 Adiabatic Tubular Reactor 493	
11.5	Adiabatic Equilibrium Conversion and Reactor Staging 11.5.1 Equilibrium Conversion 502 11.5.2 Reactor Staging 505	
11.6	Optimum Feed Temperature 509	

Xİİ Contents

CHAPTER 12 STEADY-STATE NONISOTHERMAL REACTOR DESIGN— FLOW REACTORS WITH HEAT EXCHANGE	521
12.1 Steady-State Tubular Reactor with Heat Exchange 522	321
12.1.1 Deriving the Energy Balance for a PFR 522	
12.2 Balance on the Heat Transfer Fluid 525 12.2.1 Co-Current Flow 525	
12.2.2 Counter Current Flow 526	
11 , 0	30 537
12.4 CSTR with Heat Effects 545	
12.4.1 Heat Added to the Reactor, \dot{Q} 546	
12.5 Multiple Steady States (MSS) 556	
12.5.1 Heat-Removed Term, $R(T)$ 557	
12.5.2 Heat-Generated Term, $G(T)$ 558	
12.5.3 Ignition-Extinction Curve 560	
12.6 Nonisothermal Multiple Chemical Reactions 563	
12.6.1 Energy Balance for Multiple Reactions in Plug-Flow	
Reactors 563	
12.6.2 Parallel Reactions in a PFR 564 12.6.3 Energy Balance for Multiple Reactions in a CSTR 56	. -
12.6.3 Energy Balance for Multiple Reactions in a CSTR 56 12.6.4 Series Reactions in a CSTR 567	,,
12.6.5 Complex Reactions in a PFR 570	
12.7 Safety 577	
12.7 Safety 377	
CHAPTER 13 UNSTEADY-STATE NONISOTHERMAL REACTOR DESIGNATION	N 601
13.1 The Unsteady-State Energy Balance 602	
13.2 Energy Balance on Batch Reactors 604	
13.2.1 Adiabatic Operation of a Batch Reactor 605 13.2.2 Case History of a Batch Reactor with Interrupted Isother Operation Causing a Runaway Reaction 608	rmal
13.3 Semibatch Reactors with a Heat Exchanger 615	
13.4 Unsteady Operation of a CSTR 620 13.4.1 Startup 620	
13.5 Nonisothermal Multiple Reactions 624	
APPENDIX A NUMERICAL TECHNIQUES	649
APPENDIX B IDEAL GAS CONSTANT AND CONVERSION FACTORS	655

APPENDIX C	THERMODYNAMIC RELATIONSHIPS INVOLVING THE EQUILIBRIUM CONSTANT	659
APPENDIX D	NOMENCLATURE	665
APPENDIX E	SOFTWARE PACKAGES	669
E.1 E.2 E.3	Polymath 669 E.1.A About Polymath 669 E.1.B Polymath Tutorials 670 AspenTech 670 COMSOL 671	
E.4	Software Packages 671	
APPENDIX F	RATE LAW DATA	673
APPENDIX G	OPEN-ENDED PROBLEMS	675
G.1	Design of Reaction Engineering Experiment 675	
G.2		
G.3	-	
G.4		
G.5	_	
G.6	S	
G.7		
G.8	•	
G.9	Methanol Poisoning 676	
G.10		
APPENDIX H	HOW TO USE THE DVD-ROM	679
H.1	DVD-ROM Components 679	
H.2	How the DVD-ROM/Web Can Help Learning Styles H.2.1 Global vs. Sequential Learners H.2.2 Active vs. Reflective Learners H.2.3 Sensing vs. Intuitive Learners H.2.4 Visual vs. Verbal Learners 683 683	
H.3	Navigation 683	
INDEX		685