

CONTENTS

<i>Preface</i>	ix
<i>List of Sources of Some Problems</i>	xi
<i>List of Symbols</i>	xiii
CHAPTER 1. MATHEMATICAL AND NUMERICAL METHODS	1
THEORY	
1.1 Software	1
1.2 Plotting and curvefitting	2
1.3 Regression of tabular data	2
1.4 Roots of numerical equations	3
1.5 Integration and differentiation	4
1.6 Ordinary differential equations	5
1.7 Numerical solution of ODEs	7
1.8 Partial differential equations	9
Tables	10
PROBLEMS P1.00.00	
1. Regression	15
2. Roots	18
3. Integration and differentiation	22
4. Analytical solution of ordinary differential equations	25
5. Numerical solution of ordinary differential equations	28
CHAPTER 2. REACTION RATES AND OPERATING MODES	33
Index of Reactions in Problem Section P2.02.XX	33
Index of Mechanisms in Problem Section P2.03.XX	33
THEORY	
2.1 Rate of reaction	34
2.2 Concentration, mols, partial pressure, mol fraction	35
2.3 Reaction time	36
2.4 Constants of the rate equation	36
2.5 Multiple reactions and stoichiometric balances	37
2.6 Reactor operating modes	39
2.7 Heterogeneous reactions. Rates of diffusion	41
Tables	43

PROBLEMS P2.00.00

1. Stoichiometric balances	50
2. Integrated rate equations	54
3. Complex reaction mechanisms	68
4. Numerical integrations	86

CHAPTER 3. TREATMENT OF EXPERIMENTAL DATA 94

THEORY

3.1 Kinds of laboratory reactors	94
3.2 Chemical composition	95
3.3 Power law rate equations	95
3.4 Rate equations for multiple mechanisms	97
3.5 Pressure data	99
3.6 Other properties related to composition	100
3.7 Temperature variation	100
3.8 Homogeneous catalysis	101
3.9 CSTR data. Liquid or gas phase	101
3.10 Plug flow reactors. Laminar flow	102
Figures	102a

PROBLEMS P3.00.00

1. Units	103
2. Data of chemical composition	106
3. Pressure changes	145
4. Variables related to composition	164
5. Half time and initial rate data	177
6. Temperature variation. Activation energy	187
7. Homogeneous catalysis	202
8. Enzyme and solid catalysis	210
9. Flow reactor data	222
10. CSTR data	231
11. Complex reactions	238

CHAPTER 4. IDEAL REACTORS 247

THEORY

4.1 Equilibrium constants	248
4.2 Temperature change and heat of reaction	249
4.3 Batch reactors	249
4.4 Continuous stirred tank reactors (CSTR)	250
4.5 Tubular and packed flow reactors	252
4.6 Recycle and separation modes	253
4.7 Temperature changes	253
4.8 Laminar and power law flows	254
4.9 Unsteady conditions with accumulation terms	255
4.10 Multiple steady states	256
4.11 Optima	257
4.12 Economic balance	257
Figures	258

PROBLEMS P4.00.00

1. Equilibrium constants	250
2. Temperature change and heat of reaction	276
3. Batch reactors	283
4. Continuous stirred tank reactors (CSTR)	301
5. Tubular and packed flow reactors	343
6. Recycle and separation modes	370
7. Temperature changes	383
8. Laminar and power law flows	410
9. Unsteady conditions with accumulation terms	417
10. Multiple steady states	444
11. Optima	454
12. Economic balances	471

CHAPTER 5. REACTOR EFFICIENCY 489

THEORY

5.1 Introduction	489
5.2 Tracers	490
5.3 Reactor efficiency	490
5.4 Tracer response	490
5.5 Tracer equations	494
5.6 Characterization of curves	496
5.7 Chemical conversion	498
5.8 The dispersion model	500
Figures and Tables	503

PROBLEMS P5.00.00

1. Tracer response functions	509
2. Correlations: Gamma, Gauss, etc.	531
3. Tracer response to combined elements	546
4. Conversion with known flow patterns. Laminar flow	557
5. Segregated flow, part I	568
6. Segregated flow, part II	584
7. Maximum mixed flow	602
8. Dispersion model	617

CHAPTER 6. REACTIONS WITH SOLID CATALYSTS 639

THEORY

6.1 Catalytic processes	639
6.2 Power law equations	639
6.3 Langmuir-Hinshelwood processes	640
6.4 Physical properties of granular catalysts	640
6.5 Adsorption equations	640
6.6 Extensions of the Langmuir equation	641
6.7 Rate when adsorptive equilibrium is maintained	642
6.8 Rate when chemical equilibrium is maintained	642
6.9 Find the constants of a rate equation	643
6.10 Interpretation of data	643
6.11 Several controlling steps	644
6.12 With diffusional resistance	644

Figures and Tables	646
PROBLEMS P6.00.00	
1. Physical properties of catalysts	648
2. Adsorption	652
3. Reaction mechanisms	662
4. Finding rate equations	668
5. Using rate equations	693
6. Diffusional resistance	706
 CHAPTER 7. REACTIONS WITH POROUS SOLID CATALYSTS	 719
THEORY	
7.1 Particles and pores	719
7.2 Diffusion and diffusivity	720
7.3 Equations of diffusion and reaction	722
7.4 Diffusion and reaction on nonpermeable catalysts	723
7.5 Diffusion and reaction in pores. Effectiveness	724
7.6 External and internal diffusion	725
7.7 Variable temperature	726
7.8 Deactivation of catalysts	727
 PROBLEMS P7.00.00	
1. Particles and pores	730
2. Diffusion	735
3. Concentration profiles and effectiveness	739
4. Conversion and reactor sizing	759
5. With external diffusion	770
6. Effects of temperature and deactivation	781
 CHAPTER 8. MULTIPLE PHASE REACTIONS	 798
THEORY	
8.1 Axial and radial gradients in packed beds	798
8.2 Gas-liquid reactions	801
8.3 Liquid-liquid reactions	804
8.4 Gas-liquid-solid reactions	805
8.5 Biochemical reactors	808
Figures and Tables	812
 PROBLEMS P8.00.00	
1. Packed beds	815
2. Gas-liquid reactions	828
3. Gas-liquid-solid reactions	836
4. Biochemical reactions	841
 Index of Substances	 861
Index of Subjects	865