

Table of Contents

- Chapter 1 Elements of Reaction Kinetics
 - 1.1 Definitions of Chemical Rates
 - 1.3 Coupled Reactions
 - 1.4 Reducing the Size of Kinetic Models
 - 1.6 Complex Reactions
 - 1.7 Modeling the Rate Coefficient
- Part 1 Interfacial Gradient Effects
- Part 2 Intraparticle Gradient Effects
 - 1.2 Rate Equations
 - 1.5 Bio-Kinetics
 - 2.3 Rate Equations
- Chapter 3 Transport Processes with Reactions Catalyzed by Solids
- Chapter 2 Kinetics of Heterogeneous Catalytic Reactions
 - 3.2 Mass and heat transfer resistances
 - 2.1 Introduction
 - 2.6 Model Discrimination and Parameter Estimation
 - 2.2 Adsorption on Solid Catalysts
 - 2.4 Complex Catalytic Reactions
 - 2.8 Expert Systems in Kinetics Studies
 - 3.1 Reaction of a component of a fluid at the surface of a solid
 - 2.5 Experimental Reactors
 - 3.3 Concentration or partial pressure and temperature differences
 - 2.7 Sequential Design of Experiments
 - 3.4 Molecular-, Knudsen-, and surface diffusion in pores
 - 3.5 Diffusion in a catalyst particle
 - 3.6 Diffusion and reaction in a catalyst particle. A continuum model
 - 3.7 Falsification of rate coefficient and activation energy by diffusion limitations
 - 3.8 Influence of diffusion limitations on the selectivities of coupled reactions
 - 3.9 Criteria for the importance of intraparticle diffusion limitations
 - 3.10 Multiplicity of steady states in catalyst particles
 - 3.11 Combination of external and internal diffusion limitations
 - 3.12 Diagnostic experimental criteria for the absence of internal and external mass transfer limitations
 - 3.13 Nonisothermal particles
- Chapter 4 Noncatalytic Gas-Solid Reactions
 - 4.1 A Qualitative Discussion of Gas-Solid Reactions
 - 4.2 General Model with Interfacial and Intraparticle Gradients
 - 4.3 Heterogeneous Model with Shrinking Unreacted Core
 - 4.4 Models Accounting Explicitly for the Structure of the Solid
 - 4.5 On the Use of More Complex Kinetic Equations
- Chapter 5 Catalyst Deactivation
 - 5.1 Types of Catalyst Deactivation
 - 5.2 Kinetics of Catalyst Poisoning
 - 5.3 Kinetics of Catalyst Deactivation by Coke Formation

- Chapter 6 Gas-Liquid Reactions
 - 6.1 Introduction
 - 6.2 Models for Transfer at a Gas-Liquid Interface
 - 6.3 Two-Film Theory
 - 6.4 Surface Renewal Theory
- Chapter 7 The Modeling of Chemical Reactors
 - 7.1 Approach
 - 7.2 Aspects of Mass-, Heat- and Momentum Balances
 - 7.3 The Fundamental Model Equations
- Chapter 8 The Batch and Semibatch Reactors
 - Introduction
 - 8.1 The Isothermal Batch Reactor
 - 8.2 The Nonisothermal Batch Reactor
 - 8.3 Semibatch Reactor Modeling
- Chapter 9 The Plug Flow Reactor
 - 6.5 Experimental Determination of the Kinetics of Gas-Liquid Reactions
 - 8.4 Optimal Operation Policies and Control Strategies
 - 9.1 The Continuity, Energy, and Momentum Equations
 - 9.2 Kinetic Studies Using a Tubular Reactor with Plug Flow
 - 9.3 Design and Simulation of Tubular Reactors with Plug Flow
- Chapter 10 The Perfectly Mixed Flow Reactor
 - 10.1 Introduction
 - 10.2 Mass and Energy Balances
 - 10.3 Design for Optimum Selectivity in Simultaneous Reactions
 - 10.4 Stability of Operation and Transient Behavior
- Chapter 11 Fixed Bed Catalytic Reactors
 - Part 1 Introduction
 - 11.1 The Importance and Scale of Fixed Bed Catalytic Processes
 - 11.2 Factors of Progress: Technological Innovations and Increased Fundamental Insight
 - 11.3 Factors Involved in the Preliminary Design of Fixed Bed Reactors
 - 11.4 Modeling of Fixed Bed Reactors
 - Part 2 Pseudohomogeneous Models
 - 11.5 The Basic One-Dimensional Model
 - 11.6 One-Dimensional Model with Axial Mixing
 - 11.7 Two-Dimensional Pseudohomogeneous Models
 - Part 3 Heterogeneous Models
 - 11.8 One-Dimensional Model Accounting for Interfacial Gradients
 - 11.9 One-Dimensional Model Accounting for Interfacial and Intraparticle Gradients
 - 11.10 Two-Dimensional Heterogeneous Models
- Chapter 12 Complex Flow Patterns
 - 12.1 Introduction
 - 12.2 Macro- and Micro-Mixing in Reactors
 - 12.3 Models Explicitly Accounting for Mixing
 - 12.4 Micro- Probability Density Function Methods
 - 12.5 Micro-PDF Moment Methods: Computational Fluid Dynamics

- 12.6 Macro-PDF / Residence Time Distribution Methods
- 12.7 Semi-Empirical Models for Reactors with Complex Flow Patterns
- Chapter 13 Fluidized Bed and Transport Reactors
 - 13.1 Introduction
 - 13.2 Technological Aspects of Fluidized Bed and Riser Reactors
 - 13.3 Some Features of the Fluidization and Transport of Solids
 - 13.4 Heat Transfert in Fluidized Beds
 - 13.5 Modeling of Fluidized Bed Reactors
 - 13.6 Modeling of a Transport of Riser Reactor
 - 13.7 Fluidized Bed Reactor Models Considering Detailed Flow Patterns
 - 13.8 Catalytic Cracking of Vacuum Gas Oil
- Chapter 14 Multiphase Flow Reactors
 - 14.1 Types of Multiphase Flow Reactors
 - 14.2 Design Models for Multiphase Flow Reactors
 - 14.3 Specific Design Aspects