Contents

	Preface XVII Notation XXI
1	Introduction 1
1.1	What is Chemical Technology? 1
1.2	The Chemical Industry 2
2	Chemical Aspects of Industrial Chemistry 7
2.1	Stability and Reactivity of Chemical Bonds 7
2.1.1	Factors that Influence the Electronic Nature of Bonds and Atoms
2.1.2	Steric Effects 8
2.1.3	Classification of Reagents 9
2.2	General Classification of Reactions 10
2.2.1	Acid-Base Catalyzed Reactions 11
2.2.2	Reactions via Free Radicals 11
2.2.3	Nucleophilic Substitution Reactions 13
2.2.4	Reactions via Carbocations 14
2.2.5	Electrophilic Substitution Reactions at Aromatic Compounds 15
2.2.6	Electrophilic Addition Reactions 17
2.2.7	Nucleophilic Addition Reactions 17
2.2.8	Asymmetric Synthesis 17
2.3	Catalysis 19
2.3.1	Introduction and General Aspects 20
2.3.2	Homogeneous, Heterogeneous, and Biocatalysis 26
2.3.3	Production and Characterization of Heterogeneous Catalysts 29
2.3.4	Deactivation of Catalysts 32
2.3.5	Future Trends in Catalysis Research 35
3	Thermal and Mechanical Unit Operations 39
3.1	Properties of Gases, Liquids, and Solids 40
3.1.1	Ideal and Real Gas 40
3.1.2	Heat Capacities and the Joule-Thomson Effect 45
3.1.3	Physical Transformations of Pure Substances: Vaporization and Melting 48
3.1.4	Transport Properties (Diffusivity, Viscosity, Heat Conduction) 52
3.1.4.1	Basic Equations for Transfer of Heat, Mass, and Momentum 52
3.1.4.2	Transport Coefficients of Gases 57
3.1.4.3	Transport Coefficients of Liquids 61
3.2	Heat and Mass Transfer in Chemical Engineering 65
3.2.1	Heat Transport 66
3.2.1.1	Heat Conduction 66
3.2.1.2	Heat Transfer by Convection (Heat Transfer Coefficients) 67

7



3.2.1.3	Boiling Heat Transfer 78
3.2.1.4	Heat Transfer by Radiation 79
3.2.1.5	Transient Heat Transfer by Conduction and Convection 80
3.2.2	Mass Transport 84
3.2.2.1	Forced Flow in Empty Tubes and Hydrodynamic Entrance Region 84
3.2.2.2	Steady-State and Transient Diffusive Mass Transfer 85
3.2.2.3	Diffusion in Porous Solids 89
3.3	Thermal Unit Operations 93
3.3.1	Heat Exchangers (Recuperators and Regenerators) 94
3.3.2	Distillation 97
3.3.2.1	Distillation Principles 98
3.3.2.2	Design of Distillation Columns (Ideal Mixtures) 101
3.3.2.3	Azeotropic, Extractive, and Pressure Swing Distillation 106
3.3.2.4	Reactive Distillation 108
3.3.3	Absorption (Gas Scrubbing) 108
3.3.3.1	Absorption Principles 108
3.3.3.2	Design of Absorption Columns 113
3.3.4	Liquid–Liquid Extraction 116
3.3.4.1	Extraction Principles 116
3.3.4.2	Design of Extraction Processes 118
3.3.5	Adsorption 120
3.3.5.1	Adsorption Principles 120
	Design of Adsorption Processes 130
3.3.5.2	Fluid-Solid Extraction 136
3.3.6	
3.3.6.1	1 5
3.3.6.2	Design of Fluid-Solid Extractions 139
3.3.7	Crystallization 140
3.3.7.1	Ideal Binary Eutectic Phase System 140
3.3.7.2	Ideal Binary Phase System with Both Solids Completely
	Soluble in One Another 141
3.3.8	Separation by Membranes 144
3.3.8.1	Principles of Membrane Separation 144
3.3.8.2	Applications of Membrane Separation Processes 147
3.4	Mechanical Unit Operations 151
3.4.1	Conveyance of Fluids 152
3.4.1.1	Pressure Loss in Empty Tubes 152
3.4.1.2	Pressure Loss in Fixed, Fluidized, and Entrained Beds 156
3.4.1.3	Compressors and Pumps 159
3.4.2	Contacting and Mixing of Fluids 161
3.4.3	Crushing and Screening of Solids 163
3.4.3.1	Particle Size Reduction 163
3.4.3.2	Particle Size Analysis 164
3.4.3.3	Screening and Classification of Particles (Size Separation) 166
3.4.3.4	Solid-Solid Separation (Sorting of Different Solids) 167
3.4.4	Separation of Solids from Fluids 168
3.4.4.1	Filtration 168
3.4.4.2	Separation of Solids from Fluids by Sedimentation 168
3.4.4.3	Screening and Classification of Particles (Size Separation) 171
4	Chambel Boards B. J. 1975
4	Chemical Reaction Engineering 175
4.1	Main Aspects and Basic Definitions of Chemical Reaction
4 4 -	Engineering 176
4.1.1	Design Aspects and Scale-Up Dimensions of Chemical Reactors 176
4.1.2	Speed of Chemical and Biochemical Reactions 177
4.1.3	Influence of Reactor Type on Productivity 178

4.1.4 4.1.5 4.1.6	Terms used to Characterize the Composition of a Reaction Mixture 179 Terms used to Quantify the Result of a Chemical Conversion 179 Reaction Time and Residence Time 180
4.1.7	Space Velocity and Space-Time Yield 181
4.2 4.2.1 4.2.2 4.2.3 4.2.4 4.2.5	Chemical Thermodynamics 182 Introduction and Perfect Gas Equilibria 183 Real Gas Equilibria 190 Equilibrium of Liquid–Liquid Reactions 193 Equilibrium of Gas–Solid Reactions 195 Calculation of Simultaneous Equilibria 197
4.3 4.3.1 4.3.1.1 4.3.1.2 4.3.1.3 4.3.2 4.3.2.1	Kinetics of Homogeneous Reactions 200 Rate Equation: Influence of Temperature and Reaction Order 200 First-Order Reaction 204 Reaction of n-th Order 204 Second-Order Reaction 205 Parallel Reactions and Reactions in Series 206 Two Parallel First-Order Reactions 206
4.3.2.2 4.3.3	Two First-Order Reactions in Series 207 Reversible Reactions 210
4.3.4	Reactions with Varying Volume (for the Example of a Batch Reactor) 213
4.4	Kinetics of Fluid–Fluid Reactions 216
4.4.1	Mass Transfer at a Gas-Liquid Interface (Two-Film Theory) 217
4.4.2	Mass Transfer with (Slow) Homogeneous Reaction in the Bulk Phase 219
4.4.3	Mass Transfer with Fast or Instantaneous Reaction near or at the
	Interface 220
4.5	Kinetics of Heterogeneously Catalyzed Reactions 226
4.5 4.5.1	Kinetics of Heterogeneously Catalyzed Reactions 226 Spectrum of Factors Influencing the Rate of Heterogeneously Catalyzed Reactions 227
	Spectrum of Factors Influencing the Rate of Heterogeneously Catalyzed
4.5.1	Spectrum of Factors Influencing the Rate of Heterogeneously Catalyzed Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231
4.5.1 4.5.2 4.5.2.1 4.5.2.2	Spectrum of Factors Influencing the Rate of Heterogeneously Catalyzed Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231
4.5.1 4.5.2 4.5.2.1	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235
4.5.1 4.5.2 4.5.2.1 4.5.2.2	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalysed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalysed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247 Combined Influence of Pore Diffusion and Intraparticle Heat
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4 4.5.4.1	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalysed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4 4.5.4.1 4.5.4.2	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247 Combined Influence of Pore Diffusion and Intraparticle Heat Transport 252 Simultaneous Occurrence of Interfacial and Internal Mass Transport
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4 4.5.4.1 4.5.4.2 4.5.5	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247 Combined Influence of Pore Diffusion and Intraparticle Heat Transport 252 Simultaneous Occurrence of Interfacial and Internal Mass Transport Effects 254
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4 4.5.4.1 4.5.4.2 4.5.5 4.5.5.1	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247 Combined Influence of Pore Diffusion and Intraparticle Heat Transport 252 Simultaneous Occurrence of Interfacial and Internal Mass Transport Effects 254 Irreversible First-Order Reaction 254 Reversible First-Order Reaction with the Influence of External and Internal Mass Transfer 256
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4 4.5.4.1 4.5.4.2 4.5.5 4.5.5.1 4.5.5.2	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247 Combined Influence of Pore Diffusion and Intraparticle Heat Transport 252 Simultaneous Occurrence of Interfacial and Internal Mass Transport Effects 254 Irreversible First-Order Reaction with the Influence of External and Internal Mass Transfer 256 Influence of External and Internal Mass Transfer on Selectivity 259
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4 4.5.4.1 4.5.4.2 4.5.5 4.5.5.1	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247 Combined Influence of Pore Diffusion and Intraparticle Heat Transport 252 Simultaneous Occurrence of Interfacial and Internal Mass Transport Effects 254 Irreversible First-Order Reaction 254 Reversible First-Order Reaction with the Influence of External and Internal Mass Transfer 256
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4 4.5.4.1 4.5.4.2 4.5.5 4.5.5.1 4.5.5.2	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247 Combined Influence of Pore Diffusion and Intraparticle Heat Transport 252 Simultaneous Occurrence of Interfacial and Internal Mass Transport Effects 254 Irreversible First-Order Reaction 254 Reversible First-Order Reaction with the Influence of External and Internal Mass Transfer 256 Influence of External and Internal Mass Transfer on Selectivity 259 Influence of External Mass Transfer on the Selectivity of Reactions in
4.5.1 4.5.2 4.5.2.1 4.5.2.2 4.5.3 4.5.3.1 4.5.3.2 4.5.4 4.5.4.1 4.5.4.2 4.5.5 4.5.5.1 4.5.5.2 4.5.6 4.5.6.1	Reactions 227 Chemical Reaction Rate: Surface Kinetics 231 Sorption on the Surface of Solid Catalysts 231 Rate Equations for Heterogeneously Catalyzed Surface Reactions 231 Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat 235 Interaction of External Mass Transfer and Chemical Reaction 235 Combined Influence of External Mass and Heat Transfer on the Effective Rate 239 Chemical Reaction and Internal Transport of Mass and Heat 247 Pore Diffusion Resistance and Effective Reaction Rate 247 Combined Influence of Pore Diffusion and Intraparticle Heat Transport 252 Simultaneous Occurrence of Interfacial and Internal Mass Transport Effects 254 Irreversible First-Order Reaction 254 Reversible First-Order Reaction with the Influence of External and Internal Mass Transfer 256 Influence of External and Internal Mass Transfer on Selectivity 259 Influence of External Mass Transfer on the Selectivity of Reactions in Series 259 Influence of External Mass Transfer on the Selectivity of Parallel

F.0	Kinetics of Gas-Solid Reactions 208
l.6.1	Spectrum of Factors Influencing the Rate of Gas-Solid Reactions 269
1.6.2	Reaction of a Gas with a Non-porous Solid 270
4.6.2.1	Survey of Border Cases and Models for a Reaction of a Gas with a Non-porous Solid 270
1.6.2.2	Shrinking Non-porous Unreacted Core and Solid Product Layer 270
1.6.2.3	Shrinking Non-porous Unreacted Core and Gaseous Product(s) 273
1.6.3	Reaction of a Gas with a Porous Solid 276
4.6.3.1	Survey of Border Cases and Models for a Reaction of a Gas with a Porous Solid 276
4.6.3.2	Basic Equations for the Conversion of a Porous Solid with a Gaseous Reactant 277
4.6.3.3	General Closed Solution by Combined Model (Approximation) 277
1.6.3.4	Homogeneous Uniform Conversion Model (No Concentration Gradients) 280
4.6.3.5	Shrinking Unreacted Core Model (Rate Determined by Diffusion Through Product Layer) 280
1.7	Criteria used to Exclude Interphase and Intraparticle Mass and Heat Transport Limitations in Gas-Solid Reactions and Heterogeneously Catalyzed Reactions 282
I.7.1	External Mass Transfer Through Boundary Layer 282
1.7.2	External Heat Transfer 283
1.7.3	Internal Mass Transfer 284
1.7.4	Internal Heat Transfer 284
I. 8	Kinetics of Homogeneously or Enzyme Catalyzed Reactions 287
l.8.1	Homogeneous and Enzyme Catalysis in a Single-Phase System 287
1.8.2	Homogeneous Two-Phase Catalysis 290
	·
1.9	Kinetics of Gas-Liquid Reactions on Solid Catalysts 291
1.9.1	Introduction 291
1.9.2	High Concentration of Liquid Reactant B (or pure B) and Slightly
	Soluble Gas 295
1.9.3	Low Concentration of Liquid Reactant B and Highly Soluble Gas and/or
	High Pressure 295
l.10	Chemical Reactors 296
l.10.1	Overview of Reactor Types and their Characteristics 296
4.10.1.1	Brief Outline of Ideal and Real Reactors 296
1.10.1.2	Classification of Real Reactors Based on the Mode of Operation 298
4.10.1.3	Classification of Real Reactors According to the Phases 299
1.10.2	Ideal Isothermal Reactors 305
4.10.2.1	Well-Mixed (Discontinuous) Isothermal Batch Reactor 306
4.10.2.2	Continuously Operated Isothermal Ideal Tank Reactor 307
4.10.2.3	Continuously Operated Isothermal Ideal Tubular Reactor 308
	Continuously Operated Isothermal Tubular Reactor with Laminar
	Flow 309
4.10.2.5	Continuously Operated Isothermal Cascade of Tank Reactors 311
1.10.2.6	Ideal Isothermal Tubular Recycle Reactor 311
1.10.2.7	Comparison of the Performance of Ideal Isothermal Reactors 313
l.10.3	Non-isothermal Ideal Reactors and Criteria for Prevention of Thermal
	Runaway 316
4.10.3.1	Well-Mixed (Discontinuously Operated) Non-isothermal Batch
	Reactor 317
4.10.3.2	Continuously Operated Non-isothermal Ideal Tank Reactor (CSTR) 322
4.10.3.2 4.10.3.3	· · · · · · · · · · · · · · · · · ·
r.10.J.J	Communicacy Operation 19011-150ther must fueur fueur reactor 328

4.10.3.4	Optimum Operating Lines of Continuous Ideal Non-isothermal
	Reactors 332
4.10.4	Non-ideal Flow and Residence Time Distribution 336
4.10.5	Tanks-in-Series Model 340
4.1 0 .5.1	Residence Time Distribution of a Cascade of Ideal Stirred Tank
	Reactors 340
4.10.5.2	Calculation of Conversion by the Tanks-in-Series Model 342
4.10.6	Dispersion Model 343
4.10.6.1	Axial Dispersion and Residence Time Distribution 343
4.10.6.2	Calculation of Conversion by the Dispersion Model 348
	Dispersion and Conversion in Empty Pipes 349
	Dispersion of Mass and Heat in Fixed Bed Reactors 352
4.10. 6 .5	Radial Variations in Bed Structure: Wall Effects in Narrow
	Packed Beds 354
	Modeling of Fixed Bed Reactors 355
	Fundamental Balance Equations of Fixed Bed Reactors 355
4.10.7.2	Criteria used to Exclude a Significant Influence of Dispersion in Fixed Bed
	Reactors 357
4.10.7.3	Radial Heat Transfer in Packed Bed Reactors and Methods to Account
4 10 0	for This 363
	Novel Developments in Reactor Technology 370
	Hybrid (Multifunctional) Reactors 370
	Monolithic Reactors 372
	Microreactors 373 Adiabatic Reactors with Periodic Flow Reversal 376
4.10.6.4	Adiabatic Reactors with Periodic Flow Reversal 376
4.11	Measurement and Evaluation of Kinetic Data 379
4.11.1	1 0
	Microkinetics 380
	Macrokinetics 380
	Laboratory Reactors 380
	Pros and Cons of Integral and Differential Method 382
4.11.2	,
4.11.3	•
4.11.4	1 ,
4.11.4.1	
11112	of Dispersion 389 Gradientless Ideal Particle Behavior: Criteria to Exclude the Influence
7.11.7.2	of Interfacial and Internal Transport of Mass and Heat 390
4.11.4.3	
7.11.7.3	Bed 392
4.11.5	Case Studies for the Evaluation of Kinetic Data 392
	Case Study I: Thermal Conversion of Naphthalene 392
	Case Study II: Heterogeneously Catalyzed Hydrogenation
	of Hexene 394
4.11.5.3	Case Study III: Heterogeneously Catalyzed Multiphase Reaction 395
	Case Study IV: Non-isothermal Oxidation of Carbon Nanotubes
	and Fibers 400

Raw Materials, Products, Environmental Aspects, and Costs of Chemical Technology 407 5

- Raw Materials and Energy Sources 408 5.1
- 5.1.1 Energy Consumption, Reserves and Resources of Fossil Fuels and Renewables 408
- Global and Regional Energy Consumption and Fuel Shares 408 5.1.1.1
- World Energy Consumption and World Population 410 5.1.1.2

5.1.1.3	Economic and Social Aspects of Energy Consumption 410
5.1.1.4 5.1.1.5	Conventional and Non-conventional Fossil Fuels 418 Nuclear Power 420
5.1.1.6	Renewable Energy 421
5.1.1.7	Energy Mix of the Future 422
5.1.1.8	Global Warming 425
5.1.1.9	Ecological Footprint and Energy Consumption 425
5.1.1.10	Energy Demand and Energy Mix to Reconcile the World's Pursuit of Welfare and Happiness with the Necessity to Preserve the Integrity of the Biosphere 428
5.1.2	Composition of Fossil Fuels and Routes for the Production
	of Synthetic Fuels 431
5.1.3	Natural Gas and Other Technical Gases 433
5.1.3.1	Properties of Natural Gas and Other Technical Gases 433
5.1.3.2	Conditioning of Natural Gas, Processes and Products Based
	on Natural Gas 435
5.1.4	Crude Oil and Refinery Products 437
5.1.4.1	Production, Reserves, and Price of Crude Oil 437
5.1.4.2	Properties of Crude Oil 440
5.1.4.3	Properties of Major Refinery Products 442
5.1.4.4	Refinery Processes 443
5.1.5	Coal and Coal Products 445
5.1.5.1	Properties of Coal and Other Solid Fuels 445
5.1.5.2	Processes and Products Based on Coal 447
5.1.6	Renewable Raw Materials 450
5.1.6.1	Base Chemicals from Renewable Raw Materials 450
5.1.6.2	Fats and Vegetable Oils 451
5.1.6.3	Carbohydrates 453
5.1.6.4	Extracts and Excreta from Plants 455
5.2	Inorganic Products 457
5.3	Organic Intermediates and Final Products 459
5.3.1	Alkanes and Syngas 460
5.3.2	Alkenes, Alkynes, and Aromatic Hydrocarbons 464
5.3.3	Organic Intermediates Functionalized with Oxygen, Nitrogen,
	or Halogens 472
5.3.3.1	Alcohols 472
5.3.3.2	Ethers 477
5.3.3.3	Epoxides 478
5.3.3.4	Aldehydes 478
5.3.3.5	Ketones 481
5.3.3.6	Acids 481
5.3.3.7	Amines and Nitrogen-Containing Intermediates 484
5.3.3. 8	Lactams, Nitriles, and Isocyanates 486
5.3.3.9	Halogenated Organic Intermediates 488
5.3.4	Polymers 491
5.3.4.1	Polyolefins and Polydienes 492
5.3.4.2	Vinyl-Polymers and Polyacrylates 493
5.3.4.3	Polyesters, Polyamides, and Polyurethanes 497
5.3.5	Detergents and Surfactants 500
5.3.5.1	Structure and Properties of Detergent and Surfactants 500
5.3.5.2	Cationic Detergents 501
5.3.5.3	Anionic Detergents 502
5.3.5.4	Non-ionic Detergents 504
5.3.6	Fine Chemicals 505
·	

5.3.6.1 5.3.6.2 5.3.6.3 5.3.6.4 5.3.6.5	Dyes and Colorants 506 Adhesives 506 Fragrance and Flavor Chemicals 506 Pesticides 506 Vitamins, Food, and Animal Feed Additives 508
5.3.6.6 5.4 5.4.1	Pharmaceuticals 508 Environmental Aspects of Chemical Technology 509 Air Pollution 510
5.4.2 5.4.3	Air Pollution 510 Water Consumption and Pollution 512 "Green Chemistry" and Quantifying the Environmental Impact of Chemical Processes 515
5.5 5.5.1 5.5.2 5.5.3 5.5.4	Production Costs of Fuels and Chemicals Manufacturing 517 Price of Chemical Products 517 Investment Costs 518 Variable Costs 521 Operating Costs (Fixed and Variable Costs) 522
6.1 6.1.1 6.1.2 6.1.3 6.1.4	Examples of Industrial Processes 525 Ammonia Synthesis 525 Historical Development of Haber–Bosch Process 525 Thermodynamics of Ammonia Synthesis 528 Kinetics and Mechanism of Ammonia Synthesis 529 Technical Ammonia Process and Synthesis Reactors 531
6.2 6.2.1 6.2.2 6.2.2.1 6.2.2.2 6.2.2.3 6.2.3 6.2.4	Syngas and Hydrogen 536 Options to Produce Syngas and Hydogen (Overview) 536 Syngas from Solid Fuels (Coal, Biomass) 542 Basic Principles and Reactions of Syngas Production from Solid Fuels 542 Syngas Production by Gasification of Solid Fuels 543 Case Study: Syngas and Hydrogen by Gasification of Biomass 544 Syngas by Partial Oxidation of Heavy Oils 552 Syngas by Steam Reforming of Natural Gas 555
6.3 6.3.1 6.3.2 6.3.3 6.3.4	Sulfuric Acid 558 Reactions and Thermodynamics of Sulfuric Acid Production 558 Production of SO ₂ 559 SO ₂ Conversion into SO ₃ 560 Sulfuric Acid Process 566
6.4 6.4.1 6.4.2 6.4.2.1	Nitric Acid 568 Reactions and Thermodynamics of Nitric Acid Production 568 Kinetics of Catalytic Oxidation of Ammonia 572 Catalytic Oxidation of Ammonia on a Single Pt Wire for Cross-Flow of the Gas 573
6.4.2.2 6.4.3 6.4.4	Catalytic Oxidation of Ammonia in an Industrial Reactor, that is, on a Series of Pt Gauzes 579 NO Oxidation 583 Nitric Acid Processes 584
6.5 6.5.1 6.5.1.1 6.5.1.2 6.5.2 6.5.2.1 6.5.2.2	Steel Production based on Scrap and Direct Reduced Iron (DRI) 589 Production of Blast Furnace Coke 589 Inspection of Transient Process of Coking of Coal 591 Case I: Negligible Thermal Resistance of Coal/Coke Charge 591

6.5.2.4	Case III: Thermal Resistances of Brick Wall and Coal Charge have to be Considered 594
6.5.3	Production of Pig Iron in a Blast Furnace 595
6.5.3.1	Coke Consumption of a Blast Furnace: Historical Development and Theoretical Minimum 599
6.5.3.2	Residence Time Distribution of a Blast Furnace 601
6.6	Basic Chemicals by Steam Cracking 604
6.6.1	General and Mechanistic Aspects 605
6.6.2	Factors that Influence the Product Distribution 608
6.6.2.1	Influence of Applied Feedstock 608
6.6.2.2	Influence of the Temperature in the Cracking Oven 608
6.6.2.3	Influence of Residence Time 608
6.6.2.4	Influence of Hydrocarbon Partial Pressure in the Cracking Oven 609
6.6.3	Industrial Steam Cracker Process 610
6.6.4	Economic Aspects of the Steam Cracker Process 615
6.7	Liquid Fuels by Cracking of Heavy Oils 616
6.7.1	Thermal Cracking (Delayed Coking) 616
6.7.2	Fluid Catalytic Cracking (FCC Process) 620
6.8	Clean Liquid Fuels by Hydrotreating 624
6.8.1	History, Current Status, and Perspective of Hydrotreating 624
6.8.2	Thermodynamics and Kinetics of Hydrodesulfurization (HDS) 625
6.8.3	Hydrodesulfurization Process and Reaction Engineering Aspects 629
6.9	High Octane Gasoline by Catalytic Reforming 633
6.9.1	Reactions and Thermodynamics of Catalytic Reforming 633
6.9.2	Reforming Catalyst 636
6.9.3	Process of Catalytic Reforming 637
6.9.4	Deactivation and Regeneration of a Reforming Catalyst 638
6.9.4.1	Coke Burn-Off within a Single Catalyst Particle 639
6.9.4.2	Regeneration in a Technical Fixed Bed Reactor 645
6.10	Refinery Alkylation 652
6.10.1	Reaction and Reaction Mechanism of Refinery Alkylation 652
6.10.2	Alkylation Feedstock and Products 654
6.10.3	Process Variables 655
6.10.3.1	Reaction Temperature 655
	Acid Strength and Composition 656
6.10.3.3	Isobutane Concentration 656
6.10.3.4	Effect of Mixing 656
6.10.4	Commercial Alkylation Processes 657
	Commercial Processes using Hydrofluoric Acid as Liquid Catalyst 657
6.10.4.2	Commercial Processes Using Sulfuric Acid as Liquid Catalyst 658
6.10.4.3	Comparison of Commercially Applied Alkylation Processes 661
6.11	Fuels and Chemicals from Syngas: Methanol and Fischer-Tropsch
C 11 1	Synthesis 662
6.11.1	Fischer–Tropsch Synthesis 664
6.11.1.1	· · · · · · · · · · · · · · · · · · ·
6.11.1.2	2 1 1
6.11.1.3	History, Current Status, and Perspectives of Fischer-Tropsch Synthesis 670
6.11.1.4	•
6.11.1.5	Modeling of a Multi-tubular Fixed Bed Fischer-Tropsch Reactor 677
6.11.2	Methanol Synthesis 685 Thermodynamics of Methanol Synthesis 686
6.11.2.1 6.11.2.2	Thermodynamics of Methanol Synthesis 686 Catalysts for Methanol Synthesis 689
	Catalysts for Methanol Synthesis 689 Processes and Synthesis Peactors 692

6.12 6.12.1	Ethylene and Propylene Oxide 695 Commercial Production of Ethylene Oxide 695
6.12.1.1	Chlorohydrin Process 696
	Direct Oxidation of Ethylene 696
	Products Made of Ethylene Oxide 699
6.12.2	Commercial Production of Propylene Oxide 700
	Chlorohydrin Process 700
	Indirect Oxidation of Propylene 702
6.12.2.3	Products Made of Propylene Oxide 705
6.13	Catalytic Oxidation of o-Xylene to Phthalic Acid Anhydride 706
6.13.1	Production and Use of Phthalic Anhydride (Overview) 707
6.13.2	Design and Simulation of a Multi-tubular Reactor for Oxidation
	of o-Xylene to PA 708
6.14	Hydroformylation (Oxosynthesis) 716
6.14.1	Industrial Relevance of Hydroformylation 717
6.14.2	Hydroformylation Catalysis 718
6.14.3	·
6.14.4	Advanced Catalyst Immobilization Technologies for Hydroformylation
	Catalysis 730
6.14.4.1	Immobilization of Homogeneous Hydroformylation Catalysts on Solid
	Surfaces by Covalent Anchoring 731
6.14.4.2	Catalyst Separation by Size Exclusion Membranes 732
	Catalyst Immobilization in Liquid–Liquid Biphasic Reaction Systems using
0.1 1. 7.5	Fluorous Phases, Supercritical CO ₂ or Ionic Liquids 733
6 14 4 4	Supported Liquid Hydroformylation Catalysis 736
6.15	Acetic Acid 739
6.15.1	Acetic Acid Synthesis via Acetaldehyde Oxidation 741
6.15.2	Acetic Acid Synthesis via Butane or Naphtha Oxidation 742
6.15.3	Acetic Acid Synthesis via Methanol Carbonylation 743
6.15.3.1	BASF High-Pressure Process 743
6.15.3.2	Monsanto Low-Pressure Process 744
6.15.3.3	Cativa Process 747
6.15.4	Other Technologies for the Commercial Production of Acetic Acid 747
	Direct Ethylene Oxidation 747
6.15.4.2	Acetic Acid Production by Ethane and Methane Oxidation 748
6 .16	Ethylene Oligomerization Processes for Linear 1-Alkene Production 749
6.16.1	Industrial Relevance of 1-Olefins 749
6.16.2	Aluminum-alkyl-based "Aufbaureaktion" (Growth Reaction) 750
6.16.3	Nickel-Catalyzed Oligomerization – Shell Higher Olefins Process
	(SHOP) 753
6.16.4	Metallacycle Mechanism for Selective Ethylene Oligomerization 757
6.17	Production of Fine Chemicals (Example Menthol) 763
6.17.1	Menthol and Menthol Production (Overview) 763
6.17.2	Thermodynamics and Kinetics of Epimerization of Menthol
V.11.L	Isomers 764
6.17.3	Influence of Mass Transfer on the Epimerization of Menthol
0.17.5	Isomers 766
6.17.4	Epimerization of Menthol Isomers in Technical Reactors 771
6.18	
6.18.1	Treatment of Exhaust Gases from Mobile and Stationary Sources 773 Automotive Emission Control 773
0.10.1.1	Emission Standards and Primary Measures for Reduction of Engine Emissions 773
61917	
0.10.1.2	Catalytic Converters for Reduction of Car Engine Emissions 775

6.18.2	Selective Catalytic Reduction (SCR) of NO _x from Flue Gas from Power Plants 778
6.18.2.1	Treatment of Flue Gas from Power Plants (Overview) 778
	Formation of Nitrogen Oxides during Fuel Combustion in Power Plants 779
6.18.2.3	Catalysts and Reactors for Selective Catalytic Reduction of NO _x 780
6.18.2.4	Reaction Chemistry of Selective Catalytic Reduction of NO _x 781
6.18.2.5	Reaction Kinetics and Design of SCR Reactor 781
6.19	Industrial Electrolysis 786
6.19.1	Electrochemical Kinetics and Thermodynamics 786
6.19.1.1	Faraday's Law and Current Efficiency 786
6.19.1.2	Electrochemical Potentials 787
6.19.1.3	Galvanic and Electrolysis Cells, Nernst's Law 788
6.19.1.4	Standard Electrode Potentials 789
6.19.1.5	Electrical Work and Thermoneutral Enthalpy Voltage 789
6.19.1.6	Overpotentials 791
6.19.2	Chlorine and Sodium Hydroxide 791
6.19.2.1	Applications of Chlorine and Sodium Hydroxide 791
6.19.2.2	Processes of Chlor-Alkali Electrolysis 792
6.19.2.3	Diaphragm Process 793
6.19.2.4	Mercury Cell Process 795
6.19.2.5	Membrane Process 796
6.19.3	Electrolysis of Water 797
6.19.4	Electrometallurgy (Purification of Metals by Electrorefining) 800
6.19.4.1	Electrolytic Refining in Aqueous Solution 800
6.19.4.2	Fused Salt Electrolysis (Production of Aluminum) 801
6.20	Polyethene Production 803
6.20.1	Polyethene Classification and Industrial Use 803
6.20.2	General Characteristics of PE Production Processes 805
6.20.2.1	Exothermicity of the Reaction and Thermal Stability of Ethene 805
6.20.2.2	Purity of Ethene 805
6.20.3	Reaction Meachanism and Process Equipment for the Production of LDPE 806
6.20.4	Catalysts for the Production of HDPE and LLDPE 809
6.20.4.1	Ziegler Catalyst Systems 809
	Phillips Catalyst Systems 810
6.20.4.3	
6.20.5	Production Processes for HDPE and LLDPE 812
6.20.6	PE Production Economics and Modern Developments in PE
	Production 815

References 817 Index 833