

Contents

	Preface of First Edition (and Guidelines How to Use This Textbook)	<i>xvii</i>
	Why a Second Edition?	<i>xviii</i>
	Notation	<i>xxi</i>
1	Introduction	1
1.1	What Is Chemical Technology?	1
1.2	The Chemical Industry	2
1.3	The Changing Global Economic Map	6
2	Chemical Aspects of Industrial Chemistry	19
2.1	Stability and Reactivity of Chemical Bonds	19
2.1.1	Factors that Influence the Electronic Nature of Bonds and Atoms	19
2.1.2	Steric Effects	20
2.1.3	Classification of Reagents	21
2.2	General Classification of Reactions	21
2.2.1	Acid–Base-Catalyzed Reactions	22
2.2.2	Reactions via Free Radicals	23
2.2.3	Nucleophilic Substitution Reactions	24
2.2.4	Reactions via Carbocations	24
2.2.5	Electrophilic Substitution Reactions at Aromatic Compounds	25
2.2.6	Electrophilic Addition Reactions	27
2.2.7	Nucleophilic Addition Reactions	27
2.2.8	Asymmetric Synthesis	28
2.3	Catalysis	30
2.3.1	Introduction and General Aspects	30
2.3.2	Homogeneous, Heterogeneous, and Biocatalysis	35
2.3.3	Production and Characterization of Heterogeneous Catalysts	38
2.3.4	Deactivation of Catalysts	41
2.3.5	Future Trends in Catalysis Research	43
3	Thermal and Mechanical Unit Operations	45
3.1	Properties of Gases and Liquids	46
3.1.1	Ideal and Real Gas	46
3.1.2	Heat Capacities and the Joule–Thomson Effect	50
3.1.3	Physical Transformations of Pure Substances: Vaporization and Melting	53
3.1.4	Transport Properties (Diffusivity, Viscosity, Heat Conduction)	58
3.1.4.1	Basic Equations for Transfer of Heat, Mass, and Momentum	58
3.1.4.2	Transport Coefficients of Gases	61
3.1.4.3	Transport Coefficients of Liquids	66

3.2	Heat and Mass Transfer in Chemical Engineering	69
3.2.1	Heat Transport	69
3.2.1.1	Heat Conduction	69
3.2.1.2	Heat Transfer by Convection (Heat Transfer Coefficients)	70
3.2.1.3	Boiling Heat Transfer	80
3.2.1.4	Heat Transfer by Radiation	81
3.2.1.5	Transient Heat Transfer by Conduction and Convection	82
3.2.2	Mass Transport	86
3.2.2.1	Forced Flow in Empty Tubes and Hydrodynamic Entrance Region	86
3.2.2.2	Steady-State and Transient Diffusive Mass Transfer	87
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	99
3.3.2.1	Distillation Principles	100
3.3.2.2	Design of Distillation Columns (Ideal Mixtures)	104
3.3.2.3	Azeotropic, Extractive, and Pressure Swing Distillation	108
3.3.2.4	Reactive Distillation	110
3.3.3	Absorption (Gas Scrubbing)	110
3.3.3.1	Absorption Principles	110
3.3.3.2	Design of Absorption Columns	116
3.3.4	Liquid–Liquid Extraction	118
3.3.4.1	Extraction Principles	118
3.3.4.2	Design of Extraction Processes	120
3.3.5	Adsorption	122
3.3.5.1	Adsorption Equilibrium and Adsorption Isotherms	122
3.3.5.2	Adsorption Kinetics (Single Particle)	129
3.3.5.3	Design of Adsorption Processes	131
3.3.6	Fluid–Solid Extraction	136
3.3.6.1	Principles of Fluid–Solid Extraction	136
3.3.6.2	Design of Fluid–Solid Extractions	138
3.3.7	Crystallization	139
3.3.7.1	Ideal Binary Eutectic Phase System	139
3.3.7.2	Ideal Binary Phase System with Both Solids Completely Soluble in One Another	140
3.3.8	Separation by Membranes	141
3.3.8.1	Principles of Membrane Separation	141
3.3.8.2	Applications of Membrane Separation Processes	144
3.4	Mechanical Unit Operations	149
3.4.1	Conveyance of Fluids	149
3.4.1.1	Pressure Loss in Empty Tubes	149
3.4.1.2	Pressure Loss in Fixed, Fluidized, and Entrained Beds	154
3.4.1.3	Compressors and Pumps	157
3.4.2	Contacting and Mixing of Fluids	159
3.4.3	Crushing and Screening of Solids	160
3.4.3.1	Particle Size Reduction	160
3.4.3.2	Particle Size Analysis	160
3.4.3.3	Screening and Classification of Particles (Size Separation)	164
3.4.3.4	Solid–Solid Separation (Sorting of Different Solids)	164
3.4.4	Separation of Solids from Fluids	164
3.4.4.1	Filtration	164
3.4.4.2	Separation of Solids from Fluids by Sedimentation	165
3.4.4.3	Screening and Classification of Particles (Size Separation)	167

4	Chemical Reaction Engineering	171
4.1	Main Aspects and Basic Definitions of Chemical Reaction Engineering	171
4.1.1	Design Aspects and Scale-up Dimensions of Chemical Reactors	172
4.1.2	Speed of Chemical and Biochemical Reactions	172
4.1.3	Influence of Reactor Type on Productivity	174
4.1.4	Terms Used to Characterize the Composition of a Reaction Mixture	174
4.1.5	Terms Used to Quantify the Result of a Chemical Conversion	175
4.1.6	Reaction Time and Residence Time	175
4.1.7	Space Velocity and Space–Time Yield	176
4.2	Chemical Thermodynamics	177
4.2.1	Introduction and Perfect Gas Equilibria	177
4.2.2	Real Gas Equilibria	184
4.2.3	Equilibrium of Liquid–Liquid Reactions	186
4.2.4	Equilibrium of Gas–Solid Reactions	188
4.2.5	Calculation of Simultaneous Equilibria	190
4.3	Kinetics of Homogeneous Reactions	192
4.3.1	Rate Equation: Influence of Temperature and Reaction Order	192
4.3.1.1	<i>First-Order Reaction</i>	195
4.3.1.2	<i>Reaction of nth Order</i>	196
4.3.1.3	<i>Second-Order Reaction</i>	196
4.3.2	Parallel Reactions and Reactions in Series	197
4.3.2.1	<i>Two Parallel First-Order Reactions</i>	197
4.3.2.2	<i>Two First-Order Reactions in Series</i>	197
4.3.3	Reversible Reactions	200
4.3.4	Reactions with Varying Volume (for the Example of a Batch Reactor)	203
4.4	Kinetics of Fluid–Fluid Reactions	204
4.4.1	Mass Transfer at a Gas–Liquid Interface (Two-Film Theory)	205
4.4.2	Mass Transfer with (Slow) Homogeneous Reaction in the Bulk Phase	207
4.4.3	Mass Transfer with Fast or Instantaneous Reaction near or at the Interface	208
4.5	Kinetics of Heterogeneously Catalyzed Reactions	213
4.5.1	Spectrum of Factors Influencing the Rate of Heterogeneously Catalyzed Reactions	213
4.5.2	Chemical Reaction Rate: Surface Kinetics	217
4.5.2.1	<i>Sorption on the Surface of Solid Catalysts</i>	217
4.5.2.2	<i>Rate Equations for Heterogeneously Catalyzed Surface Reactions</i>	217
4.5.3	Reaction on a Solid Catalyst and Interfacial Transport of Mass and Heat	222
4.5.3.1	<i>Interaction of External Mass Transfer and Chemical Reaction</i>	222
4.5.3.2	<i>Combined Influence of External Mass and Heat Transfer on the Effective Rate</i>	225
4.5.4	Chemical Reaction and Internal Transport of Mass and Heat	232
4.5.4.1	<i>Pore Diffusion Resistance and Effective Reaction Rate</i>	232
4.5.4.2	<i>Combined Influence of Pore Diffusion and Intraparticle Heat Transport</i>	238
4.5.5	Simultaneous Occurrence of Interfacial and Internal Mass Transport Effects	240
4.5.5.1	<i>Irreversible First-Order Reaction</i>	240
4.5.5.2	<i>Reversible First-Order Reaction with the Influence of External and Internal Mass Transfer</i>	242
4.5.6	Influence of External and Internal Mass Transfer on Selectivity	245
4.5.6.1	<i>Influence of External Mass Transfer on the Selectivity of Reactions in Series</i>	245
4.5.6.2	<i>Influence of External Mass Transfer on the Selectivity of Parallel Reactions</i>	247
4.5.6.3	<i>Influence of Pore Diffusion on the Selectivity of Reactions in Series</i>	248
4.5.6.4	<i>Influence of Pore Diffusion on the Selectivity of Parallel Reactions</i>	251
4.6	Kinetics of Gas–Solid Reactions	253
4.6.1	Spectrum of Factors Influencing the Rate of Gas–Solid Reactions	254
4.6.2	Reaction of a Gas with a Nonporous Solid	255

4.6.2.1	<i>Survey of Border Cases and Models for a Reaction of a Gas with a Nonporous Solid</i>	255
4.6.2.2	<i>Shrinking Nonporous Unreacted Core and Solid Product Layer</i>	255
4.6.2.3	<i>Shrinking Nonporous Unreacted Core and Gaseous Product(s)</i>	257
4.6.3	<i>Reaction of a Gas with a Porous Solid</i>	260
4.6.3.1	<i>Survey of Border Cases and Models for a Reaction of a Gas with a Porous Solid</i>	260
4.6.3.2	<i>Basic Equations for the Conversion of a Porous Solid with a Gaseous Reactant</i>	261
4.6.3.3	<i>General Closed Solution by Combined Model (Approximation)</i>	261
4.6.3.4	<i>Homogeneous Uniform Conversion Model (No Concentration Gradients)</i>	263
4.6.3.5	<i>Shrinking Unreacted Core Model (Rate Determined by Diffusion Through Product Layer)</i>	263
4.7	Criteria Used to Exclude Interphase and Intraparticle Mass and Heat Transport Limitations in Gas–Solid Reactions and Heterogeneously Catalyzed Reactions	265
4.7.1	External Mass Transfer Through Boundary Layer	265
4.7.2	External Heat Transfer	266
4.7.3	Internal Mass Transfer	266
4.7.4	Internal Heat Transfer	266
4.8	Kinetics of Homogeneously or Enzyme-catalyzed Reactions	269
4.8.1	Homogeneous and Enzyme Catalysis in a Single-Phase System	269
4.8.2	Homogeneous Two-Phase Catalysis	271
4.9	Kinetics of Gas–Liquid Reactions on Solid Catalysts	273
4.9.1	Introduction	273
4.9.2	High Concentration of Liquid Reactant B (or Pure B) and Slightly Soluble Gas	275
4.9.3	Low Concentration of Liquid Reactant B and Highly Soluble Gas and/or High Pressure	275
4.10	Chemical Reactors	276
4.10.1	Overview of Reactor Types and Their Characteristics	277
4.10.1.1	<i>Brief Outline of Ideal and Real Reactors</i>	277
4.10.1.2	<i>Classification of Real Reactors Based on the Mode of Operation</i>	278
4.10.1.3	<i>Classification of Real Reactors According to the Phases</i>	279
4.10.2	Ideal Isothermal Reactors	284
4.10.2.1	<i>Well-Mixed (Discontinuous) Isothermal Batch Reactor</i>	285
4.10.2.2	<i>Continuously Operated Isothermal Ideal Tank Reactor</i>	286
4.10.2.3	<i>Continuously Operated Isothermal Ideal Tubular Reactor</i>	286
4.10.2.4	<i>Continuously Operated Isothermal Tubular Reactor with Laminar Flow</i>	287
4.10.2.5	<i>Continuously Operated Isothermal Cascade of Tank Reactors</i>	290
4.10.2.6	<i>Ideal Isothermal Tubular Recycle Reactor</i>	290
4.10.2.7	<i>Comparison of the Performance of Ideal Isothermal Reactors</i>	291
4.10.3	Non-isothermal Ideal Reactors and Criteria for Prevention of Thermal Runaway	294
4.10.3.1	<i>Well-Mixed (Discontinuously Operated) Non-isothermal Batch Reactor</i>	295
4.10.3.2	<i>Continuously Operated Non-isothermal Ideal Tank Reactor (CSTR)</i>	299
4.10.3.3	<i>Continuously Operated Non-isothermal Ideal Tubular Reactor</i>	303
4.10.3.4	<i>Optimum Operating Lines of Continuous Ideal Non-isothermal Reactors</i>	306
4.10.4	Non-ideal Flow and Residence Time Distribution	310
4.10.4.1	<i>Pulse Experiment</i>	310
4.10.4.2	<i>Step Experiment</i>	311
4.10.5	Tanks-in-Series Model	313
4.10.5.1	<i>Residence Time Distribution of a Cascade of Ideal Stirred Tank Reactors</i>	313
4.10.5.2	<i>Calculation of Conversion by the Tanks-in-Series Model</i>	315
4.10.6	Dispersion Model	315
4.10.6.1	<i>Axial Dispersion and Residence Time Distribution</i>	315
4.10.6.2	<i>Calculation of Conversion by the Dispersion Model</i>	319
4.10.6.3	<i>Dispersion and Conversion in Empty Pipes</i>	321
4.10.6.4	<i>Dispersion of Mass and Heat in Fixed Bed Reactors</i>	323
4.10.6.5	<i>Radial Variations in Bed Structure: Wall Effects in Narrow Packed Beds</i>	324
4.10.7	Modeling of Fixed Bed Reactors	325
4.10.7.1	<i>Fundamental Balance Equations of Fixed Bed Reactors</i>	325

4.10.7.2	<i>Criteria Used to Exclude a Significant Influence of Dispersion in Fixed Bed Reactors</i>	327
4.10.7.3	<i>Radial Heat Transfer in Packed Bed Reactors and Methods to Account for This</i>	332
4.10.8	<i>Novel Developments in Reactor Technology</i>	336
4.10.8.1	<i>Hybrid (Multifunctional) Reactors</i>	337
4.10.8.2	<i>Monolithic Reactors</i>	338
4.10.8.3	<i>Microreactors</i>	339
4.10.8.4	<i>Adiabatic Reactors with Periodic Flow Reversal</i>	342
4.11	Measurement and Evaluation of Kinetic Data	344
4.11.1	<i>Principal Methods for Determining Kinetic Data</i>	345
4.11.1.1	<i>Microkinetics</i>	345
4.11.1.2	<i>Macrokinetics</i>	345
4.11.1.3	<i>Laboratory Reactors</i>	345
4.11.1.4	<i>Pros and Cons of Integral and Differential Method</i>	347
4.11.2	<i>Evaluation of Kinetic Data (Reaction Orders, Rate Constants)</i>	347
4.11.3	<i>Laboratory-Scale Reactors for Kinetic Measurements</i>	350
4.11.4	<i>Transport Limitations in Experimental Catalytic Reactors</i>	351
4.11.4.1	<i>Ideal Plug Flow Behavior: Criteria to Exclude the Influence of Dispersion</i>	352
4.11.4.2	<i>Gradientless Ideal Particle Behavior: Criteria to Exclude the Influence of Interfacial and Internal Transport of Mass and Heat</i>	354
4.11.4.3	<i>Criterion to Exclude the Influence of the Dilution of a Catalytic Fixed Bed</i>	355
4.11.5	<i>Case Studies for the Evaluation of Kinetic Data</i>	356
4.11.5.1	<i>Case Study I: Thermal Conversion of Naphthalene</i>	356
4.11.5.2	<i>Case Study II: Heterogeneously Catalyzed Hydrogenation of Hexene</i>	358
4.11.5.3	<i>Case Study III: Heterogeneously Catalyzed Multiphase Reaction</i>	360
4.11.5.4	<i>Case Study IV: Non-isothermal Oxidation of Carbon Nanotubes and Fibers</i>	363

5 Raw Materials, Products, Environmental Aspects, and Costs of Chemical Technology 371

5.1	Raw Materials of Industrial Organic Chemistry and Energy Sources	372
5.1.1	<i>Energy Consumption, Reserves, and Resources of Fossil Fuels and Renewables</i>	373
5.1.1.1	<i>Global and Regional Energy Consumption and Fuel Shares</i>	373
5.1.1.2	<i>World Energy Consumption and World Population</i>	380
5.1.1.3	<i>Economic and Social Aspects of Energy Consumption</i>	380
5.1.1.4	<i>Conventional and Non-conventional Fossil Fuels</i>	387
5.1.1.5	<i>Nuclear Power</i>	389
5.1.1.6	<i>Renewable Energy</i>	390
5.1.1.7	<i>Energy Mix of the Future</i>	392
5.1.1.8	<i>Global Warming</i>	395
5.1.1.9	<i>Ecological Footprint and Energy Consumption</i>	399
5.1.1.10	<i>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</i>	401
5.1.2	<i>Composition of Fossil Fuels and Routes for the Production of Synthetic Fuels</i>	403
5.1.3	<i>Natural Gas and Other Technical Gases</i>	403
5.1.3.1	<i>Properties of Natural Gas and Other Technical Gases</i>	403
5.1.3.2	<i>Conditioning of Natural Gas, Processes, and Products Based on Natural Gas</i>	406
5.1.4	<i>Crude Oil and Refinery Products</i>	410
5.1.4.1	<i>Production, Reserves, and Price of Crude Oil</i>	410
5.1.4.2	<i>Properties of Crude Oil</i>	412
5.1.4.3	<i>Properties of Major Refinery Products</i>	414
5.1.4.4	<i>Refinery Processes</i>	415
5.1.5	<i>Coal and Coal Products</i>	418
5.1.5.1	<i>Properties of Coal and Other Solid Fuels</i>	418
5.1.5.2	<i>Processes and Products Based on Coal</i>	420
5.1.6	<i>Renewable Raw Materials</i>	422
5.1.6.1	<i>Base Chemicals from Renewable Raw Materials</i>	422

5.1.6.2	<i>Fats and Vegetable Oils</i>	423
5.1.6.3	<i>Carbohydrates</i>	426
5.1.6.4	<i>Extracts and Excreta from Plants</i>	428
5.1.7	<i>Energy Consumption in Human History</i>	429
5.1.7.1	<i>Time Travel No. 1: Global Energy Consumption from 10 000 BCE Until 2010</i>	429
5.1.7.2	<i>Time Travel No. 2: From Industrial Revolution to Modern Energy Systems</i>	429
5.1.7.3	<i>Time Travel No. 3: Building of Khufu's Giant Pyramid in Ancient Egypt</i>	433
5.1.8	<i>Power-to-X and Hydrogen Storage Technologies</i>	434
5.1.8.1	<i>Hydrogen: Compressed and Cryogenic</i>	436
5.1.8.2	<i>Chemical Hydrogen Storage: General Considerations in Gaseous Compounds</i>	440
5.1.8.3	<i>Chemical Hydrogen Storage in Gaseous Compounds</i>	440
5.1.8.4	<i>Chemical Hydrogen Storage in Liquid Compounds</i>	441
5.2	Inorganic Products and Raw Materials	448
5.2.1	<i>Nonmetallic Inorganic Materials</i>	448
5.2.2	<i>Metals</i>	453
5.3	Organic Intermediates and Final Products	469
5.3.1	<i>Alkanes and Syngas</i>	469
5.3.2	<i>Alkenes, Alkynes, and Aromatic Hydrocarbons</i>	472
5.3.3	<i>Organic Intermediates Functionalized with Oxygen, Nitrogen, or Halogens</i>	479
5.3.3.1	<i>Alcohols</i>	481
5.3.3.2	<i>Ethers</i>	484
5.3.3.3	<i>Epoxides</i>	484
5.3.3.4	<i>Aldehydes</i>	485
5.3.3.5	<i>Ketones</i>	487
5.3.3.6	<i>Acids</i>	488
5.3.3.7	<i>Amines and Nitrogen-Containing Intermediates</i>	490
5.3.3.8	<i>Lactams, Nitriles, and Isocyanates</i>	491
5.3.3.9	<i>Halogenated Organic Intermediates</i>	493
5.3.4	<i>Polymers</i>	495
5.3.4.1	<i>Polyolefins and Polydienes</i>	496
5.3.4.2	<i>Vinyl Polymers and Polyacrylates</i>	497
5.3.4.3	<i>Polyesters, Polyamides, and Polyurethanes</i>	501
5.3.5	<i>Detergents and Surfactants</i>	503
5.3.5.1	<i>Structure and Properties of Detergent and Surfactants</i>	503
5.3.5.2	<i>Cationic Detergents</i>	504
5.3.5.3	<i>Anionic Detergents</i>	504
5.3.5.4	<i>Nonionic Detergents</i>	505
5.3.6	<i>Fine Chemicals</i>	507
5.3.6.1	<i>Dyes and Colorants</i>	508
5.3.6.2	<i>Adhesives</i>	508
5.3.6.3	<i>Fragrance and Flavor Chemicals</i>	508
5.3.6.4	<i>Pesticides</i>	508
5.3.6.5	<i>Vitamins, Food, and Animal Feed Additives</i>	510
5.3.6.6	<i>Pharmaceuticals</i>	510
5.4	Environmental Aspects of Chemical Technology	512
5.4.1	<i>Air Pollution</i>	512
5.4.2	<i>Water Consumption and Water Footprint</i>	515
5.4.2.1	<i>Water Sources and Water Consumption</i>	515
5.4.2.2	<i>Water Footprint and Water Availability</i>	517
5.4.3	<i>Plastic Production, Pollution, and Recycling of Plastic Waste</i>	523
5.4.3.1	<i>Global Situation</i>	523
5.4.3.2	<i>Plastic Production and Recycling of Plastic Waste in Europe</i>	526
5.4.4	<i>"Green Chemistry" and Quantifying the Environmental Impact of Chemical Processes</i>	527

5.5	Production Costs of Fuels and Chemicals Manufacturing	530
5.5.1	Price of Chemical Products	530
5.5.2	Investment Costs	530
5.5.3	Variable Costs	532
5.5.4	Operating Costs (Fixed and Variable Costs)	533
6	Examples of Industrial Processes	537
6.1	Ammonia Synthesis	537
6.1.1	Historical Development of Haber–Bosch Process	537
6.1.2	Thermodynamics of Ammonia Synthesis	539
6.1.3	Kinetics and Mechanism of Ammonia Synthesis	540
6.1.4	Technical Ammonia Process and Synthesis Reactors	542
6.2	Syngas and Hydrogen	547
6.2.1	Options to Produce Syngas and Hydrogen (Overview)	547
6.2.2	Syngas from Solid Fuels (Coal, Biomass)	551
6.2.2.1	<i>Basic Principles and Reactions of Syngas Production from Solid Fuels</i>	551
6.2.2.2	<i>Syngas Production by Gasification of Solid Fuels</i>	552
6.2.2.3	<i>Case Study: Syngas and Hydrogen by Gasification of Biomass</i>	553
6.2.3	Syngas by Partial Oxidation of Heavy Oils	560
6.2.4	Syngas by Steam Reforming of Natural Gas	562
6.3	Sulfuric Acid	565
6.3.1	Reactions and Thermodynamics of Sulfuric Acid Production	565
6.3.2	Production of SO_2	566
6.3.3	SO_2 Conversion into SO_3	567
6.3.4	Sulfuric Acid Process	572
6.4	Nitric Acid	573
6.4.1	Reactions and Thermodynamics of Nitric Acid Production	574
6.4.2	Kinetics of Catalytic Oxidation of Ammonia	576
6.4.2.1	<i>Catalytic Oxidation of Ammonia on a Single Pt Wire for Cross-Flow of the Gas</i>	577
6.4.2.2	<i>Catalytic Oxidation of Ammonia in an Industrial Reactor, That Is, on a Series of Pt Gauzes</i>	583
6.4.3	NO Oxidation	587
6.4.4	Nitric Acid Processes	588
6.5	Coke and Steel	591
6.5.1	Steel Production (Overview)	591
6.5.1.1	<i>Steel Production Based on the Blast Furnace Route</i>	592
6.5.1.2	<i>Steel Production Based on Scrap and Direct Reduced Iron (DRI)</i>	593
6.5.2	Production of Blast Furnace Coke	593
6.5.2.1	<i>Inspection of Transient Process of Coking of Coal</i>	596
6.5.2.2	<i>Case I: Negligible Thermal Resistance of Coal/Coke Charge</i>	596
6.5.2.3	<i>Case II: Negligible Thermal Resistance of Heated Brick Wall</i>	598
6.5.2.4	<i>Case III: Thermal Resistances of Brick Wall and Coal Charge Have to Be Considered</i>	598
6.5.3	Production of Pig Iron in a Blast Furnace	599
6.5.3.1	<i>Coke Consumption of a Blast Furnace: Historical Development and Theoretical Minimum</i>	603
6.5.3.2	<i>Residence Time Distribution of a Blast Furnace</i>	606
6.6	Basic Chemicals by Steam Cracking	609
6.6.1	General and Mechanistic Aspects	609
6.6.2	Factors that Influence the Product Distribution	612
6.6.2.1	<i>Influence of Applied Feedstock</i>	612
6.6.2.2	<i>Influence of the Temperature in the Cracking Oven</i>	612
6.6.2.3	<i>Influence of Residence Time</i>	612
6.6.2.4	<i>Influence of Hydrocarbon Partial Pressure in the Cracking Oven</i>	613

6.6.3	Industrial Steam Cracker Process	613
6.6.4	Economic Aspects of the Steam Cracker Process	617
6.7	Liquid Fuels by Cracking of Heavy Oils	618
6.7.1	Thermal Cracking (Delayed Coking)	619
6.7.2	Fluid Catalytic Cracking (FCC Process)	622
6.8	Clean Liquid Fuels by Hydrotreating	625
6.8.1	History, Current Status, and Perspective of Hydrotreating	625
6.8.2	Thermodynamics and Kinetics of Hydrodesulfurization (HDS)	626
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	635
6.9.3	Process of Catalytic Reforming	635
6.9.4	Deactivation and Regeneration of a Reforming Catalyst	638
6.9.4.1	<i>Coke Burn-Off Within a Single Catalyst Particle</i>	638
6.9.4.2	<i>Regeneration in a Technical Fixed Bed Reactor</i>	643
6.10	Refinery Alkylation	649
6.10.1	Reaction and Reaction Mechanism of Refinery Alkylation	649
6.10.2	Alkylation Feedstock and Products	651
6.10.3	Process Variables	651
6.10.3.1	<i>Reaction Temperature</i>	651
6.10.3.2	<i>Acid Strength and Composition</i>	652
6.10.3.3	<i>Isobutane Concentration</i>	652
6.10.3.4	<i>Effect of Mixing</i>	652
6.10.4	Commercial Alkylation Processes	652
6.10.4.1	<i>Commercial Processes Using Hydrofluoric Acid as Liquid Catalyst</i>	653
6.10.4.2	<i>Commercial Processes Using Sulfuric Acid as Liquid Catalyst</i>	654
6.10.4.3	<i>Comparison of Commercially Applied Alkylation Processes</i>	656
6.11	Fuels and Chemicals from Syngas: Methanol and Fischer–Tropsch Synthesis	657
6.11.1	Fischer–Tropsch Synthesis	658
6.11.1.1	<i>Reactions and Mechanisms of Fischer–Tropsch Synthesis</i>	659
6.11.1.2	<i>Intrinsic and Effective Reaction Rate of Fischer–Tropsch Synthesis</i>	662
6.11.1.3	<i>History, Current Status, and Perspectives of Fischer–Tropsch Synthesis</i>	663
6.11.1.4	<i>Fischer–Tropsch Processes and Reactors</i>	666
6.11.1.5	<i>Modeling of a Multi-tubular Fixed Bed Fischer–Tropsch Reactor</i>	669
6.11.2	Methanol Synthesis	676
6.11.2.1	<i>Thermodynamics of Methanol Synthesis</i>	677
6.11.2.2	<i>Catalysts for Methanol Synthesis</i>	679
6.11.2.3	<i>Processes and Synthesis Reactors</i>	682
6.12	Ethylene and Propylene Oxide	685
6.12.1	Commercial Production of Ethylene Oxide	685
6.12.1.1	<i>Chlorohydrin Process</i>	685
6.12.1.2	<i>Direct Oxidation of Ethylene</i>	686
6.12.1.3	<i>Products Made of Ethylene Oxide</i>	688
6.12.2	Commercial Production of Propylene Oxide	689
6.12.2.1	<i>Chlorohydrin Process</i>	689
6.12.2.2	<i>Indirect Oxidation of Propylene</i>	690
6.12.2.3	<i>Products Made of Propylene Oxide</i>	692
6.13	Catalytic Oxidation of <i>o</i>-Xylene to Phthalic Acid Anhydride	694
6.13.1	Production and Use of Phthalic Anhydride (Overview)	694
6.13.2	Design and Simulation of a Multi-tubular Reactor for Oxidation of <i>o</i> -Xylene to PA	695

6.14	Hydroformylation (Oxosynthesis)	701
6.14.1	Industrial Relevance of Hydroformylation	701
6.14.2	Hydroformylation Catalysis	703
6.14.3	Current Hydroformylation Catalyst and Process Technologies	706
6.14.4	Advanced Catalyst Immobilization Technologies for Hydroformylation Catalysis	714
6.14.4.1	<i>Immobilization of Homogeneous Hydroformylation Catalysts on Solid Surfaces by Covalent Anchoring</i>	714
6.14.4.2	<i>Catalyst Separation by Size Exclusion Membranes</i>	715
6.14.4.3	<i>Catalyst Immobilization in Liquid–Liquid Biphasic Reaction Systems Using Fluorous Phases: Supercritical CO₂ or Ionic Liquids</i>	715
6.14.4.4	<i>Supported Liquid Hydroformylation Catalysis</i>	718
6.15	Acetic Acid	721
6.15.1	Acetic Acid Synthesis via Acetaldehyde Oxidation	722
6.15.2	Acetic Acid Synthesis via Butane or Naphtha Oxidation	723
6.15.3	Acetic Acid Synthesis via Methanol Carbonylation	724
6.15.3.1	<i>BASF High-Pressure Process</i>	724
6.15.3.2	<i>Monsanto Low-Pressure Process</i>	725
6.15.3.3	<i>Cativa Process</i>	727
6.15.4	Other Technologies for the Commercial Production of Acetic Acid	728
6.15.4.1	<i>Direct Ethylene Oxidation</i>	728
6.15.4.2	<i>Acetic Acid Production by Ethane and Methane Oxidation</i>	728
6.16	Ethylene Oligomerization Processes for Linear 1-Alkene Production	729
6.16.1	Industrial Relevance of 1-Olefins	729
6.16.2	Aluminum-Alkyl-Based “ <i>Aufbaureaktion</i> ” (Growth Reaction)	730
6.16.3	Nickel-Catalyzed Oligomerization: Shell Higher Olefin Process (SHOP)	733
6.16.4	Metallacycle Mechanism for Selective Ethylene Oligomerization	735
6.17	Production of Fine Chemicals (Example Menthol)	740
6.17.1	Menthol and Menthol Production (Overview)	740
6.17.2	Thermodynamics and Kinetics of Epimerization of Menthol Isomers	741
6.17.3	Influence of Mass Transfer on the Epimerization of Menthol Isomers	744
6.17.4	Epimerization of Menthol Isomers in Technical Reactors	748
6.18	Treatment of Exhaust Gases from Mobile and Stationary Sources	750
6.18.1	Automotive Emission Control	750
6.18.1.1	<i>Emission Standards and Primary Measures for Reduction of Engine Emissions</i>	750
6.18.1.2	<i>Catalytic Converters for Reduction of Car Engine Emissions</i>	752
6.18.2	Selective Catalytic Reduction (SCR) of NO _x from Flue Gas from Power Plants	756
6.18.2.1	<i>Treatment of Flue Gas from Power Plants (Overview)</i>	756
6.18.2.2	<i>Formation of Nitrogen Oxides During Fuel Combustion in Power Plants</i>	757
6.18.2.3	<i>Catalysts and Reactors for Selective Catalytic Reduction of NO_x</i>	757
6.18.2.4	<i>Reaction Chemistry of Selective Catalytic Reduction of NO_x</i>	758
6.18.2.5	<i>Reaction Kinetics and Design of SCR Reactor</i>	759
6.19	Industrial Electrolysis	763
6.19.1	Electrochemical Kinetics and Thermodynamics	763
6.19.1.1	<i>Faraday's Law and Current Efficiency</i>	763
6.19.1.2	<i>Electrochemical Potentials</i>	764
6.19.1.3	<i>Galvanic and Electrolysis Cells, Nernst's Law</i>	765
6.19.1.4	<i>Standard Electrode Potentials</i>	765
6.19.1.5	<i>Electrical Work and Thermoneutral Enthalpy Voltage</i>	765
6.19.1.6	<i>Overpotentials</i>	767
6.19.2	Chlorine and Sodium Hydroxide	768
6.19.2.1	<i>Applications of Chlorine and Sodium Hydroxide</i>	768
6.19.2.2	<i>Processes of Chlor-Alkali Electrolysis</i>	769

6.19.2.3	<i>Diaphragm Process</i>	769
6.19.2.4	<i>Mercury Cell Process</i>	770
6.19.2.5	<i>Membrane Process</i>	771
6.19.3	<i>Electrolysis of Water</i>	773
6.19.4	<i>Electrometallurgy (Purification of Metals by Electrorefining)</i>	778
6.19.4.1	<i>Electrolytic Refining in Aqueous Solution</i>	778
6.19.4.2	<i>Fused Salt Electrolysis (Production of Aluminum)</i>	779
6.20	Polyethene Production	782
6.20.1	<i>Polyethene Classification and Industrial Use</i>	782
6.20.2	<i>General Characteristics of PE Production Processes</i>	783
6.20.2.1	<i>Exothermicity of the Reaction and Thermal Stability of Ethene</i>	784
6.20.2.2	<i>Purity of Ethene</i>	784
6.20.3	<i>Reaction Mechanism and Process Equipment for the Production of LDPE</i>	784
6.20.4	<i>Catalysts for the Production of HDPE and LLDPE</i>	787
6.20.4.1	<i>Ziegler Catalyst Systems</i>	787
6.20.4.2	<i>Phillips Catalyst Systems</i>	788
6.20.4.3	<i>Single-Site Metallocene Catalyst Systems</i>	788
6.20.5	<i>Production Processes for HDPE and LLDPE</i>	789
6.20.6	<i>PE Production Economics and Modern Developments in PE Production</i>	792
6.21	Titanium Dioxide	793
6.21.1	<i>Production and Use of Titanium Dioxide (Overview)</i>	793
6.21.2	<i>Sulfate Process for Production of Titanium Dioxide</i>	793
6.21.3	<i>Chloride Process for Production of Titanium Dioxide</i>	795
6.22	Silicon	796
6.22.1	<i>Production and Use of Silicon (Overview)</i>	796
6.22.2	<i>Carbothermic Reduction of Silica</i>	797
6.22.3	<i>Refining, Casting, and Crushing of Metallurgical Grade Silicon</i>	798
6.22.4	<i>Economics of the Metallurgical Grade Silicon Production</i>	798
6.22.5	<i>Production of Photovoltaic Grade Silicon by Purification of Metallurgical Grade Silicon</i>	798
6.22.5.1	<i>Production of Photovoltaic Grade Silicon by the Siemens Process</i>	798
6.22.5.2	<i>Fluidized Bed Reactor Process for Production of Photovoltaic Grade Silicon</i>	799
6.23	Polytetrafluoroethylene (PTFE)	801
6.23.1	<i>Production and Use of PTFE (Overview)</i>	801
6.23.2	<i>Process for Production of PTFE</i>	802
6.23.3	<i>Treatment of PTFE Waste</i>	802
6.23.3.1	<i>Incineration and Disposal of PTFE Waste</i>	804
6.23.3.2	<i>Reprocessing of PTFE Waste</i>	804
6.23.3.3	<i>Chemical Recycling of PTFE Waste</i>	805
6.24	Production of Amino Acids by Fermentation	807
6.24.1	<i>General Aspects</i>	807
6.24.2	<i>Overview of the Methods Applied for Industrial Amino Acid Production</i>	807
6.24.2.1	<i>Amino Acid Extraction from Protein Hydrolysates</i>	807
6.24.2.2	<i>Chemical Synthesis</i>	808
6.24.2.3	<i>Biotechnological Processes</i>	809
6.24.3	<i>Amino Acid Fermentation</i>	810
6.24.3.1	<i>Bacteria for Amino Acid Production and Strain Development</i>	810
6.24.3.2	<i>Substrates</i>	811
6.24.3.3	<i>Fermentation Process</i>	811
6.24.3.4	<i>Downstream</i>	812

References 815

Index 841