Contents

Preface — v

About the author — vii

1 Chemical technology as science — 1
   1.1 Basic principles — 1
   1.1.1 Continuous or batch? — 2
   1.1.2 Multilevel chemical processing — 4
   1.1.3 Large or small chemical plants? — 7
   1.2 Alternative production routes — 9
   1.3 Evaluation of chemical processes — 11
   1.4 Chemical process design — 12
      1.4.1 Economic aspects — 12
      1.4.2 Flow schemes — 16
      1.4.3 Sustainable and safe chemical technology: process intensification — 21
      1.4.4 Waste management — 35
      1.4.5 Conceptual process design — 37
      1.4.6 Product design — 45
      1.4.7 Patents — 47

2 Physico-chemical foundations of chemical processes — 49
   2.1 Stoichiometry — 49
   2.2 Thermodynamics — 51
   2.3 Catalysis — 55
   2.4 Kinetics — 57
   2.5 Mass transfer — 60

3 Chemical processes and unit operations — 67
   3.1 Overview of unit operations — 67
   3.2 Mechanical processes — 68
      3.2.1 Filtration — 68
      3.2.2 Cyclonic separation by gravitation — 70
   3.3 Mass transfer processes — 71
      3.3.1 Distillation — 71
      3.3.2 Extraction — 76
      3.3.3 Crystallization — 78
      3.3.4 Adsorption — 81
      3.3.5 Absorption — 83
   3.4 Chemical reactors — 87
      3.4.1 Homogeneous processes — 87
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4.2</td>
<td>Non-catalytic heterogeneous processes</td>
<td>88</td>
</tr>
<tr>
<td>3.4.3</td>
<td>Catalytic reactors</td>
<td>91</td>
</tr>
<tr>
<td>3.4.3.1</td>
<td>Two-phase catalytic reactors</td>
<td>92</td>
</tr>
<tr>
<td>3.4.3.2</td>
<td>Three-phase catalytic reactors</td>
<td>96</td>
</tr>
<tr>
<td>4.1</td>
<td>General overview</td>
<td>103</td>
</tr>
<tr>
<td>4.2</td>
<td>Feedstock for chemical process industries</td>
<td>108</td>
</tr>
<tr>
<td>4.3</td>
<td>Oil refining</td>
<td>116</td>
</tr>
<tr>
<td>4.4</td>
<td>Natural gas processing</td>
<td>122</td>
</tr>
<tr>
<td>4.5</td>
<td>Processing of coal</td>
<td>124</td>
</tr>
<tr>
<td>4.6</td>
<td>Biomass processing</td>
<td>127</td>
</tr>
<tr>
<td>5.1</td>
<td>Steam reforming of natural gas</td>
<td>137</td>
</tr>
<tr>
<td>5.2</td>
<td>Gasification</td>
<td>148</td>
</tr>
<tr>
<td>5.3</td>
<td>Water-gas shift reaction</td>
<td>153</td>
</tr>
<tr>
<td>6.1</td>
<td>General</td>
<td>157</td>
</tr>
<tr>
<td>6.2</td>
<td>Visbreaking</td>
<td>157</td>
</tr>
<tr>
<td>6.3</td>
<td>Hydrocracking</td>
<td>160</td>
</tr>
<tr>
<td>6.4</td>
<td>Fluid catalytic cracking</td>
<td>170</td>
</tr>
<tr>
<td>6.5</td>
<td>Steam cracking</td>
<td>182</td>
</tr>
<tr>
<td>7.1</td>
<td>Catalytic reforming of gasoline fractions: combining isomerization and dehydrogenation</td>
<td>191</td>
</tr>
<tr>
<td>8.1</td>
<td>Radical chlorination</td>
<td>197</td>
</tr>
<tr>
<td>8.1.1</td>
<td>Liquid-phase chlorination</td>
<td>198</td>
</tr>
<tr>
<td>8.1.2</td>
<td>Gas-phase chlorination</td>
<td>200</td>
</tr>
<tr>
<td>8.2</td>
<td>Catalytic chlorination</td>
<td>203</td>
</tr>
<tr>
<td>8.3</td>
<td>Hydrohalogenation</td>
<td>204</td>
</tr>
<tr>
<td>8.4</td>
<td>Oxychlorination</td>
<td>205</td>
</tr>
<tr>
<td>8.5</td>
<td>Fluorination</td>
<td>208</td>
</tr>
<tr>
<td>9.1</td>
<td>Oxidation of inorganic compounds</td>
<td>209</td>
</tr>
<tr>
<td>9.1.1</td>
<td>Nitric acid</td>
<td>209</td>
</tr>
<tr>
<td>9.1.2</td>
<td>Sulfuric acid</td>
<td>212</td>
</tr>
<tr>
<td>9.2</td>
<td>Oxidation of organic compounds</td>
<td>217</td>
</tr>
<tr>
<td>9.2.1</td>
<td>Heterogeneous catalytic oxidation</td>
<td>217</td>
</tr>
</tbody>
</table>
9.2.1.1 Ethylene and propylene oxide — 219
9.2.1.2 Acrylic acid — 222
9.2.1.3 Formaldehyde — 224
9.2.1.4 Maleic anhydride — 227
9.2.1.5 Phthalic anhydride — 230
9.2.1.6 Acrylonitrile — 237
9.2.2 Liquid-phase oxidation — 239
9.2.2.1 Cyclohexane oxidation — 241
9.2.2.2 Cyclohexanol oxidation — 242
9.2.2.3 Xylene oxidation to terephthalic acid — 244
9.2.2.4 Wacker process: oxidation of ethylene to acetaldehyde — 246
9.2.2.5 Synthesis of phenol and acetone by isopropylbenzene oxidation — 249
10 Hydrogenation and dehydrogenation — 253
10.1 General — 253
10.2 Ammonia synthesis — 256
10.3 Gas-phase hydrogenation — 264
10.4 Liquid-phase hydrogenation — 265
10.5 Hydrotreating — 268
10.6 Dehydrogenation — 270
10.6.1 Dehydrogenation of light alkanes — 270
10.6.2 Dehydrogenation of ethylbenzene to styrene — 276
11 Reactions involving water: hydration, dehydration, etherification, hydrolysis, and esterification — 281
11.1 Hydration and dehydration — 281
11.2 Hydrolysis — 284
11.2.1 Acid-catalyzed hydrolysis of wood — 285
11.2.2 Enzymatic hydrolysis of acyl-L-amino acids — 287
11.2.3 Hydrolysis of fatty acids triglycerides — 288
11.3 Esterification — 289
12 Alkylation — 293
12.1 Alkylation of aromatics — 293
12.2 Alkylation of olefins — 300
12.3 O-Alkylation — 306
12.4 N-Alkylation — 311
12.5 Oxyalkylation — 312
13 Reactions with CO, CO₂, and synthesis gas — 317
13.1 Carbonylation — 317
13.2 Carboxylation — 321
13.2.1 Kolbe-Schmidt synthesis — 321
13.2.2 Urea from CO₂ and ammonia — 323
13.2.3 Synthesis of melamine — 332
13.3 Methanol from synthesis gas — 336
13.4 Hydrocarbons from synthesis gas: Fischer-Tropsch synthesis — 344
13.5 Reactions of olefins with synthesis gas: hydroformylation — 357

14 Key reactions in the synthesis of intermediates: nitration, sulfation, sulfonation, alkali fusion, ketone, and aldehyde condensation — 371
14.1 Nitration — 371
14.2 Sulfation and sulfonation — 375
14.2.1 Sulfation — 375
14.2.2 Sulfonation — 378
14.3 Alkali fusion — 383
14.4 Carbonyl condensation reactions — 384
14.4.1 Condensation with aromatic compounds — 386
14.4.2 Aldol condensation — 388
14.5 Caprolactam production — 389
14.5.1 Condensation of cyclohexanone to cyclohexanone oxime and subsequent Beckmann rearrangement — 389
14.5.2 Methods for caprolactam production — 395

15 Polymerization — 401
15.1 Polymers — 401
15.2 Step-growth polymerization — 402
15.3 Polymerization process options — 407
15.3.1 Homogeneous polymerization in substance — 407
15.3.2 Homogeneous polymerization in solution — 409
15.4 Heterogeneous polymerization — 410
15.4.1 Precipitation polymerization — 410
15.4.2 Suspension and emulsion polymerization — 415

Final words — 419

Index — 421