

# Contents

**Preface to the second edition — V**

**Preface to the first edition — VII**

**Nomenclature — XV**

**1 Introduction — 1**

**2 Kinetics in reaction engineering — 4**

- 2.1 Stoichiometry of multiple reactions — 4
- 2.2 Reaction kinetics in chemical reaction engineering — 5
  - 2.2.1 General concepts — 5
  - 2.2.2 Examples of rate equations — 6

**3 Modelling of homogeneous systems — 8**

- 3.1 Mass balances for completely backmixed tank reactors: batch, semi-batch and continuous operation — 8
- 3.2 Mass balances for tubular reactors — 13
- 3.3 Energy balances of homogeneous systems — 19
  - 3.3.1 Tank reactor — 22
  - 3.3.2 Tubular plug flow reactor — 24
  - 3.3.3 Batch reactor — 25
  - 3.3.4 Semi-batch reactors — 26
- 3.4 Physical properties and correlations of homogeneous systems — 27
  - 3.4.1 Heat capacity and reaction enthalpy — 27
  - 3.4.2 Pressure drop in tubular reactors — 28
  - 3.4.3 Dispersion coefficient — 29
- 3.5 Numerical solution of homogeneous reactor models — 30
  - 3.5.1 Model structures and algorithms — 30
  - 3.5.2 Software build-up — 35

**4 Modelling of fixed beds and fluidized beds — 38**

- 4.1 Simultaneous reaction and diffusion in fluid films and porous media — 39
- 4.2 Catalytic fixed bed reactors — 42
  - 4.2.1 Models for fixed beds — 43
  - 4.2.2 Pseudo-homogeneous models for fixed beds — 44
  - 4.2.3 Heterogeneous model for fixed beds — 49
  - 4.2.4 Model equations for the bulk phase — 57
  - 4.2.5 Pressure drop in fixed beds — 61

4.3	Numerical solution of fixed bed models —	61
4.3.1	Solution of pseudo-homogeneous models —	61
4.3.2	Solution strategy of heterogeneous models —	63
4.4	Catalytic fluidized beds —	65
4.4.1	Modelling approaches to fluidized beds —	65
4.4.2	Kunii-Levenspiel model of fluidized beds —	67
4.5	Numerical solution of fluidized bed models —	71
4.6	Physical properties and correlations for catalytic two-phase systems —	73
4.6.1	Effective diffusion coefficients in a gas phase —	73
4.6.2	Mass and heat transfer coefficients around solid particles —	74
4.6.3	Mass transfer coefficients for fluidized beds —	75
<b>5</b>	<b>Modelling of three-phase systems —</b>	<b>77</b>
5.1	Mass balances of three-phase reactors —	78
5.1.1	Phase boundaries —	78
5.1.2	Liquid-phase mass balances —	80
5.1.3	Gas-phase mass balances —	83
5.1.4	Tank reactors with complete backmixing —	84
5.1.5	Catalyst particles in three-phase reactors —	85
5.1.6	Slurry reactor in the absence of mass transfer resistances —	87
5.2	Energy balances of three-phase reactors —	88
5.3	Numerical aspects —	89
<b>6</b>	<b>Modelling of gas-liquid systems —</b>	<b>92</b>
6.1	Gas-liquid contact —	94
6.2	Gas and liquid films —	96
6.2.1	Mass balances for films —	96
6.2.2	Energy balances for liquid films —	100
6.3	Gas-liquid tank reactors —	102
6.4	Gas-liquid column reactors —	103
6.5	Energy balances for gas-liquid reactors —	107
6.6	Physical properties of gas-liquid systems —	108
6.6.1	Diffusion coefficients in gas and liquid —	108
6.6.2	Gas-liquid equilibrium —	112
6.7	Numerical strategies for gas-liquid reactor models —	113
<b>7</b>	<b>Structured reactors —</b>	<b>118</b>
7.1	Modelling principles and model equations —	120
7.2	Case study: oxidation of alcohols in microreactor —	126

<b>8</b>	<b>Modelling of unsteady-state reactor systems — 128</b>
8.1	Kinetics and transport phenomena under transient conditions — 129
8.2	Reactor modelling in case of transient kinetics — 132
8.2.1	Gas- and liquid-phase mass balances — 132
8.2.2	Adsorbed surface species — 136
8.2.3	Model summary — 136
8.3	Case study: enantioselective hydrogenation of an organic compound — 137
<b>9</b>	<b>Equipment and models for laboratory experiments — 140</b>
9.1	Homogeneous batch reactor — 140
9.2	Homogeneous stirred tank reactor (CSTR) — 144
9.3	Catalytic fixed bed in integral mode — 145
9.4	Catalytic differential reactor — 146
9.5	Catalytic gradientless reactor — 147
9.6	Catalytic slurry reactor — 148
9.7	Classification of laboratory reactor models — 148
9.7.1	Algebraic and differential models — 149
9.7.2	Linearity and nonlinearity of the model — 149
<b>10</b>	<b>Parameter estimation in reaction engineering — 152</b>
10.1	Principles of nonlinear regression analysis — 152
10.2	Statistical and sensitivity analysis of parameters — 156
10.3	Suppression of correlation between parameters — 160
10.3.1	Correlation in rate expressions — 161
10.3.2	Correlation in temperature dependencies — 163
10.4	Systematic deviations and normalization of experimental data — 165
10.5	Direct integral method — 170
10.6	Parameter estimation from non-isothermal data — 174
10.7	Estimation of parameters from semibatch experiments — 178
10.7.1	Composite reactions in the presence of a heterogeneous catalyst — 178
10.7.2	Composite reactions in the presence of a homogeneous catalyst — 182

## References — 185

## Exercises

I	Gas-phase tube reactor — 191
II	Synthesis of maleic acid monoester in a semi-batch reactor — 192
III	Exothermic reaction in a continuous stirred tank reactor — 193
IV	Production of phthalic anhydride in a fixed bed reactor — 194

V	Water-gas shift in a fixed bed reactor: diffusional limitations —	<b>196</b>
VI	Steady-state CSTR's in series: oxidation of Iron(II) to Iron(III) —	<b>198</b>
VII	A fluidized bed reactor —	<b>200</b>
VIII	Three-phase slurry reactor: hydrogenation of aromatics —	<b>201</b>
IX	Chlorination of p-cresol in a continuous stirred tank reactor —	<b>203</b>
X	Reaction between methanol and triphenyl methyl chloride —	<b>204</b>
XI	Use of millireactor for the kinetic study of very fast reaction: dehydrochlorination of 1,3-dichloro-2-propanol —	<b>205</b>
XII	Multiple liquid-phase reaction system —	<b>207</b>
XIII	Gas-liquid reactions in a semi-batch reactor —	<b>211</b>
XIV	Gas-phase reaction in a differential reactor —	<b>213</b>
XV	Three-phase reactions in a semi-batch reactor —	<b>216</b>
XVI	Non-isothermal liquid phase reaction in a CSTR —	<b>219</b>
XVII	Oxidation of sulphur dioxide in an optimal multi-bed reactor system —	<b>221</b>
XVIII	Modelling of a monolith channel —	<b>222</b>
XIX	Heterogeneous two-dimensional model for a catalytic fixed-bed reactor —	<b>223</b>
XX	Dissolution of a solid particle in a batch reactor —	<b>224</b>

## **Appendices**

### **Appendix A**

**Numerical strategies in the solution of nonlinear algebraic equations and ordinary differential equations — 227**

### **Appendix B**

**Computer simulation of CSTR, PFR and batch reactor models — 235**

### **Appendix C**

**Numerical simulation of non-isothermal tubular reactors — 243**

**Index — 249**