

Contents

Preface — V

Part I: General part

- 1 Introduction. How to describe complex processes using simple models: Modelics — 3**
 - 1.1 Model... modeling... — 3
 - 1.2 Top-down and bottom-up — 4
- 2 Categorization of models — 6**
 - 2.1 Physical framework of model design — 6
 - 2.1.1 Models of transport — 7
 - 2.1.2 The batch reactor — 8
 - 2.1.3 The continuous stirred-tank reactor — 8
 - 2.1.4 The plug-flow reactor — 9
 - 2.1.5 The pulse reactor — 10
 - 2.2 How to simplify complex models? Principles of simplification — 10
 - 2.2.1 Physicochemical assumptions of simplification of chemico-mathematical models — 11
 - 2.3 Mathematical concepts of simplification in chemical kinetics — 15
 - 2.3.1 Mathematical status of the quasi-steady-state (QSS) approximation — 15
 - 2.3.2 Limits of simplification: optimal model — 17

Part II: Chemical modelics

- 3 Basic models of chemical kinetics — 21**
 - 3.1 Equations of chemical kinetics and a scheme of parametric analysis — 21
 - 3.1.1 Experimental background — 21
 - 3.1.2 Equations of chemical kinetics — 23
 - 3.1.3 Scheme of parametric analysis — 25
 - 3.2 Autocatalytic models — 32
 - 3.2.1 Autocatalytic trigger — 32
 - 3.2.2 Autocatalytic oscillators — 34
 - 3.2.3 Association reaction — 59
 - 3.3 Catalytic schemes of transformations — 63

3.3.1	Catalytic triggers — 63
3.3.2	Catalytic oscillators — 72
3.4	Catalytic continuous stirred-tank reactor (CSTR) — 84
3.4.1	Flow reactor with an autocatalytic trigger — 86
3.4.2	Flow reactor with a catalytic trigger — 89
3.4.3	Flow reactor with an autocatalytic oscillator — 93
3.4.4	Flow reactor with a catalytic oscillator — 93
3.4.5	Kinetic “chaos” induced by noise — 94
3.5	Two-center mechanisms — 96
3.5.1	Oscillator–trigger model — 96
3.5.2	Oscillator–oscillator model — 99
3.5.3	Model with a step of interaction of centers $Z_1 \rightleftharpoons Z_2$ — 101
3.5.4	Model with a diffusion change of interaction centers — 102
3.6	Simplest models of CO oxidation on platinum — 106
3.7	Nonideal kinetics — 113
3.8	Savchenko’s model — 124
3.9	Model of the Belousov–Zhabotinsky reaction — 130
4	Thermokinetic models — 142
4.1	Continuous stirred-tank reactors (CSTR) — 142
4.2	Zel’dovich–Semenov model — 143
4.2.1	Reaction $A \rightarrow P$ — 144
4.2.2	The oxidation reaction $A + O_2 \rightarrow P$ — 152
4.2.3	Reaction $nA \rightarrow P$ — 157
4.2.4	Reaction $A \rightarrow P$ with arbitrary kinetics — 162
4.2.5	Semenov diagram as a stability criterion — 164
4.3	Aris–Amundson model — 168
4.3.1	Reaction $A \rightarrow P$ — 168
4.3.2	Reaction of the n -th order — 181
4.3.3	The oxidation reaction — 183
4.3.4	Reaction with arbitrary kinetics — 186
4.3.5	Andronov–Hopf bifurcations — 189
4.3.6	Safe and unsafe boundaries of regions of critical phenomena — 194
4.4	Volter–Salnikov model — 197
4.5	Models of a continuous stirred tank reactor and a tube reactor — 205
4.5.1	Parametric analysis of a dimensional model — 206
4.5.2	Relation between dimensionless and dimensional models — 214
4.5.3	Determination of ignition boundaries — 215
4.5.4	Continuous tube reactor — 216
4.6	Combustion model of hydrocarbon mixture — 218
4.7	Thermocatalytic triggers and oscillators — 228
4.7.1	The Eley–Rideal monomolecular mechanism — 231

4.7.2	The Eley–Rideal bimolecular mechanism —	233
4.7.3	The linear catalytic cycle —	235
4.7.4	The Langmuir–Hinshelwood Mechanism —	235
4.7.5	Autocatalytic schemes of transformations —	237
4.7.6	Autocatalytic oscillator —	245
4.8	Parallel scheme —	248
4.9	Consistent scheme —	252
4.10	One reversible reaction —	255
4.11	Model of spontaneous combustion of brown-coal dust —	259
4.12	Modeling of the nitration of amyl in a CSTR and a tube reactor —	266
4.12.1	Parametric analysis of the mathematical model of a CSTR —	267
4.12.2	Model of a tube reactor —	272
5	Models of macrokinetics —	281
5.1	Homogeneous–heterogeneous reaction —	282
5.2	Model of an imperfectly stirred continuous reactor —	287
5.3	Dissipative structures on the active surface —	291
5.4	The model of sorption–reaction–diffusion —	299
5.5	Macrokinetics of catalytic reactions on surfaces of various geometries —	307
5.6	Nonlinear interaction between the active surface and bulk of a solid —	311
5.7	Models of wave propagation reactions —	315
5.8	Macroclusters on the catalyst surface at the CO oxidation on Pt —	319
5.9	Model of coking the feed channels of the fuel —	322

Part III: Modelics everywhere

6	Models of population dynamics: “prey–predator” models —	335
6.1	“Prey–predator” model —	335
6.1.1	Nonlinearity of reproduction —	336
6.1.2	Competition in the prey population —	337
6.1.3	Saturation of the predator —	337
6.1.4	Competition for the predator —	338
6.1.5	Competition of the prey and saturation of the predator —	338
6.1.6	Nonlinearity of eating of the prey by the predator and saturation of the predator —	339
6.1.7	Competition of the predator for the prey and saturation of the predator —	340
6.1.8	Nonlinearity of reproduction of predator and competition of prey —	340

6.1.9	Saturation of the predator, nonlinearity of eating of prey by the predator, and competition of the prey —	341
6.1.10	Saturation of the predator, competition of the predator for the prey, and competition of prey —	341
6.1.11	Three populations —	346
6.1.12	One-predator–two-prey and one-prey–two-predator systems —	347
6.1.13	Community: two-prey–one-predator —	348
6.2	A mathematical model of immunology —	349
6.3	One model of economic dynamics —	351
6.4	Environmental management model —	357

Conclusion —	361
---------------------	------------

Index —	363
----------------	------------