

Contents

Part I Model Construction Problems

Simple Process Models	3
1 Mechanics of Continuous Media	4
1.1 Scalar and Vector Fields	5
1.2 Stress Tensor and Tensor Field	7
2 Hydrodynamic Processes	11
2.1 Basic Equations	11
2.2 Cylindrical Coordinates	15
2.3 Boundary Conditions	16
2.4 Laminar Boundary Layer	17
2.5 Two-Phase Boundary Layers	19
2.6 Particular Processes	22
2.7 Generalized Variables	23
2.8 Basic Parameters	25
2.9 Rheology	26
2.10 Turbulence	29
3 Mass and Heat Transfer Processes	38
3.1 Basic Equations	39
3.2 Boundary Conditions	41
3.3 Transfer Processes Rate	42
3.4 Diffusion Boundary Layer	43
3.5 Turbulent Diffusion	45
3.6 Turbulent Mass Transfer	47
4 Chemical Processes and Adsorption	49
4.1 Stoichiometry	49
4.2 Mechanism and Reaction Route	49
4.3 Kinetics of Simple Chemical Reactions	50
4.4 Kinetics of Complex Reactions	52
4.5 Adsorption Processes	53
4.6 Physical Adsorption	54

4.7	Chemical Adsorption	54
4.8	Heterogeneous Reactions	55
5	Examples	56
5.1	Dissolution of a Solid Particle	56
5.2	Contemporary Approach of Turbulence Modeling	58
	References	59
	Complex Process Models	61
1	Mechanism and Mathematical Description	61
1.1	Mechanism of Physical Absorption	62
1.2	Mathematical Description	62
1.3	Generalized Variables and Characteristic Scales	63
1.4	Dimensionless Parameters and Process Mechanism	64
1.5	Boundary Conditions and Mechanism	66
1.6	Kinetics and Mechanism	66
2	Theoretical Models: Mass Transfer in Film Flows	68
2.1	Film with a Free Interface	68
2.2	Effect of a Chemical Reaction	70
2.3	Effect of Gas Motion	70
2.4	Absorption of Slightly Soluble Gas	76
2.5	Absorption of Highly Soluble Gas	78
3	Diffusion-Type Models	81
3.1	Mass Transfer with a Chemical Reaction	81
3.2	Interphase Mass Transfer	82
3.3	Average Concentration Models	83
3.4	Airlift Reactor	86
4	Similarity Theory Models	91
4.1	Absorption in a Packed-Bed Column	92
4.2	Generalized (Dimensionless) Variables	92
4.3	Generalized Individual Case and Similarity	94
4.4	Mathematical Structure of the Models	95
4.5	Dimension Analysis	98
4.6	Some Errors in Criteria Models	100
5	Regression Models	103
5.1	Regression Equations	104
5.2	Parameter Identification	104
5.3	Least-Squares Method	104
6	Examples	105
6.1	Effect of Surfactants	105
6.2	Effect of Interface Waves	112
6.3	Photobioreactor Model	116
	References	125

Mass Transfer Theories	127
1 Linear Mass Transfer Theory	127
1.1 Model Theories	128
1.2 Boundary Layer Theory	130
1.3 Two-Phase Boundary Layers	132
2 Mass Transfer in Countercurrent Flows	134
2.1 Velocity Distribution	135
2.2 Concentration Distribution	137
2.3 Comparison Between Co-current and Countercurrent Flows	139
3 Nonlinear Mass Transfer	140
3.1 Influence of Intensive Mass Transfer on the Hydrodynamics	141
3.2 Boundary Conditions of the Nonlinear Mass Transfer Problem	143
3.3 Nonlinear Mass Transfer in the Boundary Layer	145
3.4 Two-Phase Systems	148
3.5 Nonlinear Mass Transfer and the Marangoni Effect	157
4 Examples	162
4.1 Heat Transfer in the Conditions of Nonlinear Mass Transfer	163
4.2 Multicomponent Mass Transfer	165
4.3 Concentration Effects	169
4.4 Influence of High Concentration on the Mass Transfer Rate	173
4.5 Nonlinear Mass Transfer in Countercurrent Flows	180
References	181

Part II Theoretical Analysis of Models

Qualitative Analysis	187
1 Generalized Analysis	187
1.1 Generalized Variables	187
1.2 Mass Transfer with a Chemical Reaction	188
1.3 Nonstationary Processes	190
1.4 Steady-State Processes	190
1.5 Effect of the Chemical Reaction Rate	191
2 Mechanism of Gas-Liquid Chemical Reactions	192
2.1 Irreversible Chemical Reactions	192
2.2 Homogeneous Catalytic Reactions	202
2.3 Reversible Chemical Reactions	205
2.4 Relationships Between the Chemical Equilibrium and the Physical Equilibrium During Absorption	208
3 Comparative Qualitative Analysis for Process Mechanism Identification	210
3.1 Comparison of the Nonlinear Effects	211
3.2 Nonstationary Absorption Mechanism	221

3.3	Nonstationary Evaporation Kinetics	228
4	Example	236
4.1	Sulfuric Acid Alkylation Process in a Film Flow Reactor	236
	References	240
	Quantitative Analysis	243
1	Scale-Up	243
1.1	Similarity and Scale-Up	244
1.2	Scale Effect	249
1.3	Diffusion Model	251
1.4	Scale-Up Theory	253
1.5	Axial Mixing	254
1.6	Evaluation of the Scale Effect	256
1.7	Hydrodynamic Modeling	257
2	Average Concentration Model and Scale-Up	259
2.1	Diffusion-Type Model	259
2.2	Influence of the Radial Nonuniformity of the Velocity Distribution on the Process Efficiency	260
2.3	Scale Effect	263
2.4	Average Concentration Model	264
2.5	Scale Effect Modeling	266
2.6	Scale-Up Parameter Identification	267
3	Statistical Analysis	268
3.1	Basic Terms	269
3.2	Statistical Treatment of Experimental Data	281
3.3	Estimates of the Expectation and the Dispersion	282
3.4	Tests of Hypotheses	284
3.5	Dispersion Analysis	287
3.6	Significance of Parameter Estimates and Model Adequacy . . .	289
3.7	Model Suitability	292
3.8	Adequacy of the Theoretical Models and Model Theories . . .	293
4	Example	295
4.1	Statistical Analysis of Diffusion Type Models	295
	References	296
	Stability Analysis	297
1	Stability Theory	297
1.1	Evolution Equations	297
1.2	Bifurcation Theory	301
1.3	Eigenvalue Problems	305
2	Hydrodynamic Stability	306
2.1	Fundamental Equations	306
2.2	Power Theory	307
2.3	Linear Theory	309

2.4	Stability, Bifurcations, and Turbulence	311
2.5	Stability of Parallel Flows	313
3	Orr–Sommerfeld Equation	314
3.1	Parallel Flows	315
3.2	Almost Parallel Flows	316
3.3	Linear Stability and Nonlinear Mass Transfer	316
4	Self-Organizing Dissipative Structures	328
4.1	Nonlinear Mass Transfer in the Boundary Layer	330
4.2	Gas Absorption	338
4.3	Liquid Evaporation	368
5	Examples	386
5.1	Gas–Liquid System	386
5.2	Liquid–Liquid System	389
5.3	Effect of Concentration	393
5.4	Effect of Temperature	397
	References	399

Part III Calculation Problems

	Solution of Differential Equations	405
1	Analytical Methods	405
1.1	Green’s Functions	405
1.2	Similarity Variables Method	409
1.3	Eigenvalue Problem	410
1.4	Laplace Transformation	412
2	Perturbation Methods	414
2.1	Expansions with Respect to a Parameter	414
2.2	Expansions with Respect to a Coordinate	417
2.3	Nonuniform Expansions (Poincaré–Lighthill–Ho Method)	418
3	Numerical Methods	422
3.1	Finite Differences Method	422
3.2	Finite Elements Method	423
4	Examples	424
4.1	Application of Green’s Functions	424
4.2	Sturm–Liouville Problem	425
	References	426

	Parameter Identification (Estimation)	429
1	Inverse Problems	429
1.1	Direct and Inverse Problems	430
1.2	Types of Inverse Problems	430
1.3	Incorrectness of the Inverse Problems	432

2	Sets and Metric Spaces	433
2.1	Metrics	433
2.2	Linear Spaces	434
2.3	Functional	436
2.4	Operator	436
2.5	Functional of the Misfit	437
2.6	Some Properties of the Direct and Inverse Operators.	439
3	Incorrectness of the Inverse Problems	440
3.1	Correctness After Hadamard	441
3.2	Correctness After Tikhonov	442
4	Methods for Solving Incorrect (Ill-Posed) Problems	442
4.1	Method of Selections	444
4.2	Method of Quasi-Solutions	444
4.3	Method of Substitution of Equations	445
4.4	Method of the Quasi-Reverse	445
4.5	Summary	445
5	Methods for Solving Essentially Ill-Posed Problems	446
5.1	Regularization Operator	446
5.2	Variational Approach	447
5.3	Iterative Approach	449
6	Parameter Identification in Different Types of Models	456
6.1	Regression Models	456
6.2	Selection Methods	458
6.3	Variational Regularization	459
6.4	Similarity Theory Models	461
6.5	Diffusion-Type Models	461
6.6	Theoretical Models and Model Theories	464
7	Minimum of the Least-Squares Function	465
7.1	Incorrectness of the Inverse Problem	465
7.2	Incorrectness of the Least Squares Function Method	466
7.3	Regularization of the Iterative Method for Parameter Identification	469
7.4	Iteration Step Determination and Iteration Stop Criterion	471
7.5	Iterative Algorithm	471
7.6	Correct Problem Solution	472
7.7	Effect of the Regularization Parameter	473
7.8	Incorrect Problem Solution	473
7.9	Essentially Incorrect Problem Solution	475
7.10	General Case	477
7.11	Statistical Analysis of Model Adequacy	478
7.12	Comparison between Correct and Incorrect Problems	480
8	Multiequation Models	483
8.1	Problem Formulation	484
8.2	Fermentation System Modeling	486

9	Experiment Design	494
9.1	Experimental Plans of Modeling	494
9.2	Parameter Identification	495
9.3	Significance of Parameters	498
9.4	Adequacy of Models	498
9.5	Randomized Plans	499
9.6	Full and Fractional Factor Experiment	501
9.7	Compositional Plans	504
10	Examples	505
10.1	Regression Models	505
10.2	Statistical Analysis of the Parameter Significance and Model Adequacy of the Regression Models	510
10.3	Clapeyron and Antoin Models	514
10.4	Incorrectness Criterion	515
10.5	Increase of the Exactness of the Identification Problem Solution	516
10.6	Incomplete Experimental Data Cases	518
	References	528
	Optimization	531
1	Analytical Methods	531
1.1	Unconstraints Minimization	531
1.2	Constraints Minimization	532
1.3	Calculus of Variations	533
1.4	Solution of a Set of Nonlinear Equations	536
2	Numerical Methods	537
2.1	Linear Programming	537
2.2	Nonlinear Programming	538
3	Dynamic Programming and the Principle of the Maximum	543
3.1	Functional Equations	543
3.2	Principle of Optimality	543
3.3	Principle of the Maximum	544
4	Examples	546
4.1	Problem of Optimal Equipment Change	546
4.2	A Calculus of Variations Problem	548
	References	549

Part IV Chemical Plant Systems

	Systems Analysis	553
1	Simulation of Chemical Plant Systems	553
1.1	Model of Chemical Plant Systems	554
1.2	Simulation Methods	555

1.3	Sequential Module (Hierarchical) Approach	555
1.4	Acyclic Chemical Plant Systems.	556
1.5	Cyclic Chemical Plant Systems.	558
1.6	Independent Contours	558
1.7	Breaking Sets	561
1.8	Optimal Order	562
2	Simulation for Specified Outlet Variables	563
2.1	Zone of Influence	564
2.2	Absolutely Independent Influence	566
2.3	Independent Influence	566
2.4	Combined Zones.	568
3	Models of Separate Blocks	568
3.1	Types of Modules	569
3.2	Heat Transfer	570
3.3	Separation	571
3.4	Chemical Processes	573
	References	573
	Synthesis of Systems	575
1	Optimal Synthesis of Chemical Plants	575
1.1	Optimization.	575
1.2	Optimal Synthesis.	575
1.3	Main Problems	576
1.4	Methods of Synthesis	577
1.5	Optimal Synthesis of a System for Recuperative Heat Transfer	578
2	Renovation of Chemical Plant Systems.	581
2.1	Mathematical Description.	582
2.2	Mathematical Models	584
2.3	Main Problems	585
2.4	Renovation by Optimal Synthesis of Chemical Plant Systems.	586
2.5	Renovation by Introduction of Highly Intensive Equipment . . .	587
2.6	Renovation by Introduction of Highly Effective Processes . . .	587
	References	588
	Conclusion	589
	Index	591