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Chemical Engineering Dynamics

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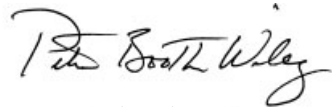
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Chemical Engineering Dynamics

An Introduction to Modelling and Computer Simulation

Third, Completely Revised Edition



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The background picture was directly taken from MADONNA, the program provided with this book, in the foreground, a batch reactor is shown with kindly permission of Pete Csiszar.
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Contents

Preface XIII

Nomenclature XVII

1 Basic Concepts

- 1.1 Modelling Fundamentals 1
 - 1.1.1 Chemical Engineering Modelling 1
 - 1.1.2 General Aspects of the Modelling Approach 3
 - 1.1.3 General Modelling Procedure 3
- 1.2 Formulation of Dynamic Models 4
 - 1.2.1 Material Balance Equations 4
 - 1.2.2 Balancing Procedures 6
 - 1.2.2.1 Case A: Continuous Stirred-Tank Reactor 7
 - 1.2.2.2 Case B: Tubular Reactor 7
 - 1.2.2.3 Case C: Coffee Percolator 8
 - 1.2.3 Total Material Balances 16
 - 1.2.3.1 Case A: Tank Drainage 17
 - 1.2.4 Component Balances 18
 - 1.2.4.1 Case A: Waste Holding Tank 19
 - 1.2.4.2 Case B: Extraction from a Solid by a Solvent 20
 - 1.2.5 Energy Balancing 22
 - 1.2.5.1 Case A: Continuous Heating in an Agitated Tank 27
 - 1.2.5.2 Case B: Heating in a Filling Tank 28
 - 1.2.5.3 Case C: Parallel Reaction in a Semi-Continuous Reactor with Large Temperature Changes 29
 - 1.2.6 Momentum Balances 31
 - 1.2.7 Dimensionless Model Equations 31
 - 1.2.7.1 Case A: Continuous Stirred-Tank Reactor (CSTR) 32
 - 1.2.7.2 Case B: Gas-Liquid Mass Transfer to a Continuous Tank Reactor with Chemical Reaction 34
- 1.3 Chemical Kinetics 35
 - 1.3.1 Rate of Chemical Reaction 35
 - 1.3.2 Reaction Rate Constant 38

1.3.3	Heat of Reaction	39
1.3.4	Chemical Equilibrium and Temperature	39
1.3.5	Yield, Conversion and Selectivity	39
1.3.6	Microbial Growth Kinetics	41
1.4	Mass Transfer Theory	43
1.4.1	Stagewise and Differential Mass Transfer Contacting	43
1.4.2	Phase Equilibria	45
1.4.3	Interphase Mass Transfer	46
2	Process Dynamics Fundamentals	
2.1	Signal and Process Dynamics	51
2.1.1	Measurement and Process Response	51
2.1.1.1	First-Order Response to an Input Step-Change Disturbance	51
2.1.1.2	Case A: Concentration Response of a Continuous Flow, Stirred Tank	52
2.1.1.3	Case B: Concentration Response in a Continuous Stirred Tank with Chemical Reaction	54
2.1.1.4	Case C: Response of a Temperature Measuring Element	55
2.1.1.5	Case D: Measurement Lag for Concentration in a Batch Reactor	57
2.1.2	Higher Order Responses	58
2.1.2.1	Case A: Multiple Tanks in Series	58
2.1.2.2	Case B: Response of a Second-Order Temperature Measuring Element	60
2.1.3	Pure Time Delay	61
2.1.4	Transfer Function Representation	62
2.2	Time Constants	63
2.2.1	Common Time Constants	64
2.2.1.1	Flow Phenomena	64
2.2.1.2	Diffusion–Dispersion	65
2.2.1.3	Chemical Reaction	65
2.2.1.4	Mass Transfer	65
2.2.1.5	Heat Transfer	67
2.2.2	Application of Time Constants	67
2.3	Fundamentals of Automatic Control	68
2.3.1	Basic Feedback Control	68
2.3.2	Types of Controller Action	69
2.3.2.1	On/Off Control	70
2.3.2.2	Proportional Integral Derivative (PID) Control	70
2.3.2.3	Case A: Operation of a Proportional Temperature Controller	72
2.3.3	Controller Tuning	73
2.3.3.1	Trial and Error Method	74
2.3.3.2	Ziegler–Nichols Open-Loop Method	74
2.3.3.3	Cohen–Coon Controller Settings	75
2.3.3.4	Ultimate Gain Method	75
2.3.3.5	Time Integral Criteria	76

2.3.4	Advanced Control Strategies	76
2.3.4.1	Cascade Control	76
2.3.4.2	Feedforward Control	77
2.3.4.3	Adaptive Control	78
2.3.4.4	Sampled Data or Discrete Control Systems	78
2.4	Numerical Aspects of Dynamic Behaviour	79
2.4.1	Optimisation	79
2.4.1.1	Case A: Optimal Cooling for a Reactor with an Exothermic Reversible Reaction	79
2.4.2	Parameter Estimation	81
2.4.2.1	Non-Linear Systems Parameter Estimation	82
2.4.2.2	Case B: Estimation of Rate and Equilibrium Constants in a Reversible Esterification Reaction Using MADONNA	83
2.4.3	Sensitivity Analysis	85
2.4.4	Numerical Integration	88
2.4.5	System Stability	91
3	Modelling of Stagewise Processes	
3.1	Introduction	93
3.2	Stirred-Tank Reactors	93
3.2.1	Reactor Configurations	93
3.2.2	Generalised Model Description	95
3.2.2.1	Total Material Balance Equation	95
3.2.2.2	Component Balance Equation	95
3.2.2.3	Energy Balance Equation	95
3.2.2.4	Heat Transfer to and from Reactors	96
3.2.2.5	Steam Heating in Jackets	99
3.2.2.6	Dynamics of the Metal Jacket Wall	100
3.2.3	The Batch Reactor	102
3.2.3.1	Case A: Constant-Volume Batch Reactor	103
3.2.4	The Semi-Batch Reactor	104
3.2.4.1	Case B: Semi-Batch Reactor	106
3.2.5	The Continuous Stirred-Tank Reactor	106
3.2.5.1	Case C: Constant-Volume Continuous Stirred-Tank Reactor	109
3.2.6	Stirred-Tank Reactor Cascade	109
3.2.7	Reactor Stability	110
3.2.8	Reactor Control	115
3.2.9	Chemical Reactor Safety	117
3.2.9.1	The Runaway Scenario	118
3.2.9.2	Reaction Calorimetry	118
3.2.10	Process Development in the Fine Chemical Industry	119
3.2.11	Chemical Reactor Waste Minimisation	120
3.2.12	Non-Ideal Flow	123
3.2.13	Tank-Type Biological Reactors	124
3.2.13.1	The Batch Fermenter	126

3.2.13.2	The Chemostat	126
3.2.13.3	The Feed Batch Fermenter	128
3.3	Stagewise Mass Transfer	129
3.3.1	Liquid–Liquid Extraction	129
3.3.1.1	Single Batch Extraction	130
3.3.1.2	Multisolute Batch Extraction	132
3.3.1.3	Continuous Equilibrium Stage Extraction	133
3.3.1.4	Multistage Countercurrent Extraction Cascade	136
3.3.1.5	Countercurrent Extraction Cascade with Backmixing	137
3.3.1.6	Countercurrent Extraction Cascade with Slow Chemical Reaction	139
3.3.1.7	Multicomponent Systems	140
3.3.1.8	Control of Extraction Cascades	141
3.3.1.9	Mixer-Settler Extraction Cascades	142
3.3.1.10	Staged Extraction Columns	149
3.3.1.11	Column Hydrodynamics	152
3.3.2	Stagewise Absorption	153
3.3.3	Stagewise Distillation	156
3.3.3.1	Simple Overhead Distillation	156
3.3.3.2	Binary Batch Distillation	158
3.3.3.3	Continuous Binary Distillation	162
3.3.3.4	Multicomponent Separations	165
3.3.3.5	Plate Efficiency	166
3.3.3.6	Complex Column Simulations	167
3.3.4	Multicomponent Steam Distillation	168
4	Differential Flow and Reaction Applications	
4.1	Introduction	173
4.1.1	Dynamic Simulation	173
4.1.2	Steady-State Simulation	174
4.2	Diffusion and Heat Conduction	175
4.2.1	Unsteady-State Diffusion	175
4.2.2	Unsteady-State Heat Conduction and Diffusion in Spherical and Cylindrical Coordinates	178
4.2.3	Steady-State Diffusion	179
4.3	Tubular Chemical Reactors	180
4.3.1	The Plug-Flow Tubular Reactor	181
4.3.2	Liquid-Phase Tubular Reactors	185
4.3.3	Gas-Phase Tubular Reactors	186
4.3.4	Batch Reactor Analogy	189
4.3.5	Dynamic Simulation of the Plug-Flow Tubular Reactor	190
4.3.6	Dynamics of an Isothermal Tubular Reactor with Axial Dispersion	193
4.3.6.1	Dynamic Difference Equation for the Component Balance Dispersion Model	193

4.3.7	Steady-State Tubular Reactor Dispersion Model	196
4.4	Differential Mass Transfer	199
4.4.1	Steady-State Gas Absorption with Heat Effects	199
4.4.1.1	Steady-State Design	200
4.4.1.2	Steady-State Simulation	201
4.4.2	Dynamic Modelling of Plug-Flow Contactors: Liquid–Liquid Extraction Column Dynamics	202
4.4.3	Dynamic Modelling of a Liquid–Liquid Extractor with Axial Mixing in Both Phases	205
4.4.4	Dynamic Modelling of Chromatographic Processes	207
4.4.4.1	Axial Dispersion Model for a Chromatography Column	208
4.4.4.2	Dynamic Difference Equation Model for Chromatography	209
4.5	Heat Transfer Applications	213
4.5.1	Steady-State Tubular Flow with Heat Loss	213
4.5.2	Single-Pass, Shell-and-Tube, Countercurrent-Flow Heat Exchanger	214
4.5.2.1	Steady-State Applications	214
4.5.2.2	Heat Exchanger Dynamics	215
4.6	Difference Formulae for Partial Differential Equations	219
4.7	References Cited in Chapters 1 to 4	220
4.8	Additional Books Recommended	222
5	Simulation Tools and Examples of Chemical Engineering Processes	
5.1	Simulation Tools	226
5.1.1	Simulation Software	226
5.1.2	Teaching Applications	227
5.1.3	Introductory MADONNA Example: BATSEQ-Complex Reaction Sequence	227
5.2	Batch Reactor Examples	232
5.2.1	BATSEQ – Complex Batch Reaction Sequence	232
5.2.2	BATCHD – Dimensionless Kinetics in a Batch Reactor	235
5.2.3	COMPREAC – Complex Reaction	237
5.2.4	BATCOM – Batch Reactor with Complex Reaction Sequence	240
5.2.5	CASTOR – Batch Decomposition of Acetylated Castor Oil	243
5.2.6	HYDROL – Batch Reactor Hydrolysis of Acetic Anhydride	247
5.2.7	OXIBAT – Oxidation Reaction in an Aerated Tank	250
5.2.8	RELUY – Batch Reactor of Luyben	253
5.2.9	DSC – Differential Scanning Calorimetry	258
5.2.10	ESTERFIT – Esterification of Acetic Acid with Ethanol. Data Fitting	261
5.3	Continuous Tank Reactor Examples	265
5.3.1	CSTRCOM – Isothermal Reactor with Complex Reaction	265
5.3.2	DEACT – Deactivating Catalyst in a CSTR	268
5.3.3	TANK and TANKDIM – Single Tank with Nth-Order Reaction	270

5.3.4	CSTRPULSE – Continuous Stirred-Tank Cascade Tracer Experiment	273
5.3.5	CASCSEQ – Cascade of Three Reactors with Sequential Reactions	276
5.3.6	REXT – Reaction with Integrated Extraction of Inhibitory Product	280
5.3.7	THERM and THERMPLOT – Thermal Stability of a CSTR	283
5.3.8	COOL – Three-Stage Reactor Cascade with Countercurrent Cooling	287
5.3.9	OSCIL – Oscillating Tank Reactor Behaviour	290
5.3.10	REFRIG1 and REFRIG2 – Auto-Refrigerated Reactor	295
5.3.11	REVTEMP – Reversible Reaction with Variable Heat Capacities	299
5.3.12	REVREACT – Reversible Reaction with Temperature Effects	305
5.3.13	HOMPOLY Homogeneous Free-Radical Polymerisation	310
5.4	Tubular Reactor Examples	315
5.4.1	TUBE and TUBEDIM – Tubular Reactor Model for the Steady State	315
5.4.2	TUBETANK – Design comparison for Tubular and Tank Reactors	317
5.4.3	BENZHYD – Dehydrogenation of Benzene	320
5.4.4	ANHYD – Oxidation of O-Xylene to Phthalic Anhydride	324
5.4.5	NITRO – Conversion of Nitrobenzene to Aniline	329
5.4.6	TUBDYN – Dynamic Tubular Reactor	332
5.4.7	DISRE – Isothermal Reactor with Axial Dispersion	335
5.4.8	DISRET – Non-Isothermal Tubular Reactor with Axial Dispersion	340
5.4.9	VARMOL – Gas-Phase Reaction with Molar Change	344
5.5	Semi-Continuous Reactor Examples	347
5.5.1	SEMIPAR – Parallel Reactions in a Semi-Continuous Reactor	347
5.5.2	SEMISEQ – Sequential-Parallel Reactions in a Semi-Continuous Reactor	350
5.5.3	HMT – Semi-Batch Manufacture of Hexamethylenetetramine	353
5.5.4	RUN Relief of a Runaway Polymerisation Reaction	355
5.5.5	SELCONT Optimized Selectivity in a semi-continuous reactor	362
5.5.6	SULFONATION Space-Time-Yield and Safety in a Semi-Continuous Reactor	365
5.6	Mixing-Model Examples	374
5.6.1	NOCSTR – Non-Ideal Stirred-Tank Reactor	374
5.6.2	TUBEMIX – Non-Ideal Tube-Tank Mixing Model	378
5.6.3	MIXFLO1 and MIXFLO2 – Mixed-Flow Residence Time Distribution Studies	381
5.6.4	GASLIQ1 and GASLIQ2 – Gas-Liquid Mixing and Mass Transfer in a Stirred Tank	385
5.6.5	SPBEDRTD – Spouted Bed Reactor Mixing Model	390

5.6.6	BATSEG, SEMISEG and COMPSEG – Mixing and Segregation in Chemical Reactors	394
5.7	Tank Flow Examples	406
5.7.1	CONFLO 1, CONFLO 2 and CONFLO 3 – Continuous Flow Tank	406
5.7.2	TANKBLD – Liquid Stream Blending	409
5.7.3	TANKDIS – Ladle Discharge Problem	412
5.7.4	TANKHYD – Interacting Tank Reservoirs	416
5.8	Process Control Examples	420
5.8.1	TEMPCONT – Control of Temperature	420
5.8.2	TWOTANK – Two Tank Level Control	424
5.8.3	CONTUN – Controller Tuning Problem	427
5.8.4	SEMIEX – Temperature Control for Semi-Batch Reactor	430
5.8.5	TRANSIM – Transfer Function Simulation	435
5.8.6	THERMFF – Feedforward Control of an Exothermic CSTR	437
5.9	Mass Transfer Process Examples	442
5.9.1	BATEX – Single Solute Batch Extraction	442
5.9.2	TWOEX – Two-Solute Batch Extraction with Interacting Equilibria	444
5.9.3	EQEX – Simple Equilibrium Stage Extractor	447
5.9.4	EQMULTI – Continuous Equilibrium Multistage Extraction	449
5.9.5	EQBACK – Multistage Extractor with Backmixing	453
5.9.6	EXTRACTCON – Extraction Cascade with Backmixing and Control	456
5.9.7	HOLDUP – Transient Holdup Profiles in an Agitated Extractor	459
5.9.8	KLADYN, KLAFIT and ELECTFIT – Dynamic Oxygen Electrode Method for K_{La}	462
5.9.9	AXDISP – Differential Extraction Column with Axial Dispersion	468
5.9.10	AMMONAB – Steady-State Design of a Gas Absorption Column with Heat Effects	471
5.9.11	MEMSEP – Gas Separation by Membrane Permeation	475
5.9.12	FILTWASH – Filter Washing	479
5.9.13	CHROMDIFF – Dispersion Rate Model for Chromatography Columns	483
5.9.14	CHROMPLATE – Stagewise Linear Model for Chromatography Columns	486
5.10	Distillation Process Examples	490
5.10.1	BSTILL – Binary Batch Distillation Column	490
5.10.2	DIFDIST – Multicomponent Differential Distillation	494
5.10.3	CONSTILL – Continuous Binary Distillation Column	496
5.10.4	MCSTILL – Continuous Multicomponent Distillation Column	501
5.10.5	BUBBLE – Bubble Point Calculation for a Batch Distillation Column	504
5.10.6	STEAM – Multicomponent, Semi-Batch Steam Distillation	508

5.11	Heat Transfer Examples	511
5.11.1	HEATEX – Dynamics of a Shell-and-Tube Heat Exchanger	511
5.11.2	SSHEATEX – Steady-State, Two-Pass Heat Exchanger	515
5.11.3	ROD – Radiation from Metal Rod	518
5.12	Diffusion Process Examples	521
5.12.1	DRY – Drying of a Solid	521
5.12.2	ENZSPLIT – Diffusion and Reaction: Split Boundary Solution	525
5.12.3	ENZDYN – Dynamic Diffusion with Enzymatic Reaction	529
5.12.4	BEAD – Diffusion and Reaction in a Spherical Catalyst Bead	533
5.13	Biological Reaction Examples	538
5.13.1	BIOREACT – Process Modes for a Bioreactor	538
5.13.2	INHIBCONT – Continuous Bioreactor with Inhibitory Substrate	543
5.13.3	NITBED – Nitrification in a Fluidised Bed Reactor	547
5.13.4	BIOFILM – Biofilm Tank Reactor	551
5.13.5	BIOFILT – Biofiltration Column for Removing Ketone from Air	555
5.14	Environmental Examples	560
5.14.1	BASIN – Dynamics of an Equalisation Basin	560
5.14.2	METAL – Transport of Heavy Metals in Water Column and Sediments	565
5.14.3	OXSAG – Classic Streeter-Phelps Oxygen Sag Curves	569
5.14.4	DISCHARGE – Dissolved Oxygen and BOD Steady-State Profiles Along a River	572
5.14.5	ASCSTR – Continuous Stirred Tank Reactor Model of Activated Sludge	577
5.14.6	DEADFISH – Distribution of an Insecticide in an Aquatic Ecosystem	581
5.14.7	LEACH – One-Dimensional Transport of Solute Through Soil	584
5.14.8	SOIL – Bioremediation of Soil Particles	591
	Appendix	597
1	A Short Guide to MADONNA	597
2	Screenshot Guide to BERKELEY-MADONNA	602
3	List of Simulation Examples	606
	Subject Index	609

Preface

The aim of this book is to teach the use of modelling and simulation as a discipline for the understanding of chemical engineering processes and their dynamics. This is done via a combination of basic modelling theory and computer simulation examples, which are used to emphasise basic principles and to demonstrate the cause-and-effect phenomena in complex models. The examples are based on the use of a powerful and easy-to-use simulation language, called BERKELEY-MADONNA, that was already successfully used in the second edition of this book. Developed at the University of California for Windows and Macintosh, MADONNA represents almost all we have ever wanted in simulation software for teaching. The many programmed examples demonstrate simple modelling procedures that can be used to represent a wide range of chemical and chemical engineering process phenomena. The study of the examples, by direct computer experimentation, has been shown to lead to a positive improvement in the understanding of physical systems and confidence in the ability to deal with chemical rate processes. Quite simple models can often give realistic representations of process phenomena. The methods described in the text are applicable to a range of differing applications, including process identification, the analysis and design of experiments, process design and optimisation, process control and plant safety, all of which are essential aspects of modern chemical technology.

The book is based on the hands-on use of the computer as an integral part of the learning process. Although computer-based modelling procedures are now commonplace in chemical engineering, our experience is that there still remains a considerable lack of ability in basic modelling, especially when applied to dynamic systems. This has resulted from the traditional steady state approach to chemical engineering and the past emphasis on flow-sheeting for large-scale continuous processes. Another important contributing factor is the perceived difficulty in solving the large sets of simultaneous differential equations that result from any realistic dynamic modelling description. With modern trends towards more intensive high-value batch processing methods, the need for a better knowledge of the plant dynamics is readily apparent. This is also reinforced by the increased attention that must now be paid to proper process control, process optimisation and plant safety. Fortunately the PC and Macintosh computers with suitable simulation software now provide a fast and convenient means of solution.

The excellent software BERKELEY-MADONNA enables a more modern, Windows-based (also Macintosh compatible) and menu driven solution.

In this third edition we have revised the theoretical part and introduced a number of new simulation examples. Some examples deal with safety problems in chemical reactors and others are related to modelling of environmental systems and are located in a new Environmental Process section.

Organisation of the Book

The book consists of an introduction to basic modelling presented in Chapters 1 to 4. An introduction to simulation principles and methods and the simulation examples are found in Chapter 5. The first four chapters cover the basic theory for the computer simulation examples and present the basic concepts of dynamic modelling. The aim is not to be exhaustive, but simply to provide sufficient introduction, for a proper understanding of the modelling methodology and computer-based examples. Here the main emphasis is placed on understanding the physical meaning and significance of each term in the resulting model equations. Chapter 5, constituting the main part of the book, provides the MADONNA-based computer simulation exercises. Each of the examples is self-contained and includes a model description, the model equations, exercises, nomenclature, sample graphical output and references. The combined book thus represents a synthesis of basic theory and computer-based simulation examples. The accompanying CD includes the MADONNA simulation language for Windows and Macintosh and the ready-to-run simulation example programs. Each program is clearly structured with comments and complete nomenclature. Although not included within the main body of the text, the MADONNA solution programs provided on the CD are very simple both to write and to understand, as evidenced by the demonstration program BATSEQ in Section 5.1.3. All the programs are clearly structured and are accompanied by clear descriptions, nomenclature and details of any special items of programming that might be included. All programs are therefore very easy to understand, to apply and, if needed, to modify. Further, a clear connection between the model relationships described in the text and the resulting program is very apparent.

Chapter 1 deals with the basic concepts of modelling, and the formulation of mass and energy balance relationships. In combination with other forms of relationship, these are shown to lead to a systematic development for dynamic models. Though the concepts are simple, they can be applied equally well to very complex problems.

Chapter 2 is employed to provide a general introduction to signal and process dynamics, including the concept of process time constants, process control, process optimisation and parameter identification. Other important aspects of dynamic simulation involve the numerical methods of solution and the resulting stability of solution; both of which are dealt with from the viewpoint of the simulator, as compared to that of the mathematician.

Chapter 3 concerns the dynamic characteristics of stagewise types of equipment, based on the concept of the well-stirred tank. In this, the various types of stirred-tank chemical reactor operation are considered, together with allowance for heat effects, non-ideal flow, control and safety. Also included is the modelling of stagewise mass transfer applications, based on liquid-liquid extraction, gas absorption and distillation.

Chapter 4 concerns differential processes, which take place with respect to both time and position and which are normally formulated as partial differential equations. Applications include heterogeneous catalysis, tubular chemical reactors, differential mass transfer, heat exchangers and chromatography. It is shown that such problems can be solved with relative ease, by utilising a finite-differencing solution technique in the simulation approach.

Chapter 5 comprises the computer simulation examples. The exercises are intended to draw the simulators attention to the most important features of each example. Most instructive is to study the influence of important model parameters, using the interactive and graphical features of MADONNA. Interesting features include the possibility of making “parametric runs” to investigate the influence of one parameter on the steady state values. When working with arrays to solve multistage or diffusion problems, the variables can be plotted versus the array number, thus achieving output plots as a function of a distance measure.

Working through a particular example will often suggest an interesting variation, such as a control loop, which can then be inserted into the model. In running our courses, the exercises have proven to be very open-ended and in tackling them, we hope you will share our conviction that computer simulation is fun, as well as being useful and informative. An Appendix provides an instructional guide to the MADONNA software, which is sufficient for work with the simulation examples.

In this edition some of our favourite examples from our previous book “Environmental Bioprocesses” have been added in a new section of Chapter 5. Also the exercises from some examples have been expanded, according to our teaching experience in the area of reactor safety and control.

We are confident that the book will be useful to all who wish to obtain a better understanding of chemical engineering dynamics and to those who have an interest in sharpening their modelling skills. We hope that teachers with an interest in modelling will find this to be a useful textbook for chemical engineering and applied chemistry courses, at both undergraduate and postgraduate levels.

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Nomenclature for Chapters 1–4

Symbols		Units
A	Area	m^2
A	Magnitude of controller input signal	various
a	Specific interfacial area	m^2/m^3 and cm^2/cm^3
a	Various parameters	various
B	Magnitude of controller output signal	various
b	Various parameters	various
C	Concentration	kg/m^3 , $kmol/m^3$
c_p	Heat capacity at constant pressure	$kJ/kg\ K$, $kJ/mol\ K$
c_v	Heat capacity at constant volume	$kJ/kg\ K$, $kJ/mol\ K$
D	Diffusivity	m^2/s
d	Differential operator	–
d, D	Diameter	m
E	Energy	kJ or kJ/kg
E	Activation energy	kJ/mol
E	Residence time distribution	–
F	Residence time distribution	–
F	Volumetric flow rate	m^3/s
f	Frequency in the ultimate gain method	1/s
G	Gas or light liquid flow rate	m^3/s
g	Gravitational acceleration	m/s^2
G'	Superficial light phase velocity	m/s
H	Enthalpy	kJ/mol , kJ/kg
ΔH	Enthalpy change	kJ/mol , kJ/kg
H	Height	m
H	Henry's law constant	$bar\ m^3/kg$
H_G	Rate of heat gain	kJ/s
H_L	Rate of heat loss	kJ/s
h	Fractional holdup	–
h_i	Partial molar enthalpy	kJ/mol
J	Total mass flux	kg/s , $kmol/s$
j	Mass flux	$kg/m^2\ s$, $mol/m^2\ s$

K	Constant in Cohen-Coon method	various
K	Mass transfer coefficient	m/s
K	kinetic growth constant	s ⁻¹
k	Constant	various
k _d	specific death rate coefficient	s ⁻¹
K _{Ga}	Gas-liquid mass transfer coefficient referring to concentration in G-phase	1/s
k _{Ga}	Gas film mass transfer coefficient	1/s
K _{La}	Gas-liquid mass transfer coefficient referring to concentration in L-phase	1/s
k _{La}	Liquid film mass transfer coefficient	1/s
K _{LX} a	Overall mass transfer capacity coefficient based on the aqueous phase mole ratio X	kmol/m ³ s
K _P	Proportional controller gain constant	various
K _s	saturation constant	kg m ⁻³
L	Length	m
L	Liquid or heavy phase flow rate	m ³ /s, mol/s
L'	Superficial heavy phase velocity	m/s
M	Mass	kg, mol
\dot{M}	Mass flow rate	kg/s
m	maintenance factor	kg S/kg X
N	Mass flux	kg/m ² s
N	Molar flow rate	mol/s
n	Number of moles	–
n	Reaction order	–
P	Controller output signal	various
P	Total pressure or pure component vapour pressure	bar
p	Partial pressure	bar
Pe	Peclet number (L v/D)	–
Q	Heat transfer rate	kJ/s
Q	Total transfer rate	kg/s, mol/s
q	Heat flux	kJ/m ² s
R	Ideal gas constant	bar m ³ /K mol
R	Reaction rate	kg/s, kmol/s
R	Number of reactions	–
r	Reaction rate	kg/m ³ s, kmol/m ³ s
r _{Ads}	Adsorption rate of the sorbate	g/cm ³ s
r _d	death rate	kg m ⁻³ s ⁻¹
r _i	Reaction rate of component i	kg i/m ³ s, kmol/m ³ s
r _Q	Heat production rate	kJ/m ³ s
r _S	Rate of substrate uptake	kg S m ⁻³ s ⁻¹
r _X	Growth rate	kg biomass/m ³ h
S	Slope of process reaction curve/A	various
S	Selectivity	–

S	Number of compounds	–
S	Concentration of substrate	kg/m ³
s	Laplace operator	–
T	Temperature	°C, K
t	Time	h, min, s
Tr _A	Transfer rate of sorbate	g/s
U	Heat transfer coefficient	kJ/m ² K s
U	Internal energy	kJ/mol
V	Vapour flow rate	mol/s
V	Volume	m ³
v	Flow velocity	m/s
W	Rate of work	kJ/s
W	Mass flow rate	kg/s
X	Concentration in heavy phase	kg/m ³ , mol/m ³
X	Mole ratio in the heavy phase	–
X	Conversion	–
X	Biomass concentration	kg/m ³
x	Mole fraction in heavy phase	–
x	Input variable	various
Y	Fractional yield	–
Y	Concentration in light phase	kg/m ³ , mol/m ³
Y	Mole ratio in the light phase	–
Y	Yield coefficient	kg/kg
Y _{i/j}	Yield of i from j	kg i/kg j
y	Mole fraction in light phase	–
y	Output variable	various
Z	Arrhenius constant	various
Z	Length variable	m
z	Length variable	m

Greek

Δ	Difference operator	–
Φ	Thiele modulus	–
Θ	Dimensionless time	–
Σ	Summation operator	–
α	Backmixing factor	–
α	Relative volatility	–
α, β	Reaction order	–
ε	Controller error	various
η	Effectiveness factor	–
η	Plate efficiency	–
μ	Dynamic viscosity	kg m/s
μ	Specific growth rate	1/h

μ_m	Maximum growth rate	1/h
ν	Stoichiometric coefficient	–
θ	Dimensionless temperature	–
ρ	Density	kg/m ³
τ	Controller time constant	s
τ	Residence time	h and s
τ	Shear stress	kg m/s ²
τ	Time constant	h, min, s
τ_L	Time lag	h, min, s
∂	Partial differential operator	–

Indices

0	Refers to initial, inlet, external, or zero order
1	Refers to outlet or first order
1, 2, ..., n	Refers to segment, stage, stream, tank or volume element
A	Refers to component A
a	Refers to ambient
abs	Refers to absorption
agit	Refers to agitation
app	Refers to apparent
avg	Refers to average
B	Refers to component B, base, backmixing, surface position or boiler
C	Refers to component C or combustion
c	Refers to cross-sectional or cold
D	Refers to derivative control, component D, delay or drum
E	Refers to electrode
eq	Refers to equilibrium
F	Refers to formation or feed
f	Refers to final or feed plate
G	Refers to gas or light liquid phase or generation
h	Refers to hot
ht	Refers to heat transfer
I	Refers to integral control
i	Refers to component i or to interface
inert	Refers to inert component
j	Refers to reaction j or to jacket
L	Refers to liquid phase, heavy liquid phase or lag
m	Refers to metal wall or mixer
max	Refers to maximum
mix	Refers to mixer
mt	Refers to mass transfer
n	Refers to tank, section, segment or plate number
p	Refers to plug flow, pocket and particle

Q	Refers to heat
R	Refers to recycle stream
r	Refers to reactor
S	Refers to settler, steam, solid or surroundings
s	Refers to surface, settler or shell side
SL	Refers to liquid film at solid interface
ss	Refers to steady state
St	Refers to standard
t	Refers to tube
tot	Refers to total
V	Refers to vapour
w	Refers to water or wall
–	Bar above symbol refers to dimensionless variable
'	Refers to perturbation variable, superficial velocity or stripping section
*	Refers to equilibrium concentration

