Chemical Engineering Dynamics

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An Introduction to Modelling and Computer Simulation

Second, Completely Revised Edition

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Also of Interest

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I. J. Dunn, E. Heinzle, J. Ingham, J. E. Přenosil
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Dynamics of Environmental Bioprocesses
Modelling and Simulation
J. B. Snape, I. J. Dunn, J. Ingham, J. E. Přenosil
1995. ISBN 3-527-28705-1

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. In this second edition the examples are based on the use of a new, powerful and easy-to-use simulation language, called Berkeley Madonna. Developed for Windows and Macintosh at the University of California, 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 of 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.

In producing this new edition, the major change is, of course, the use of Madonna as the means of solution to the model equations. This enables a more modern, Windows-based (also Macintosh compatible) and menu driven solution. Also, the increased power and speed of solution have allowed us to

extend the scope of our simulation examples quite substantially. In particular, the use of dynamic simulation as a means of making a steady-state analysis to study the variation in the steady-state conditions with changing system parameters is now possible. Regarding the text, we have included several new topics, including chemical waste minimisation, chemical reactor safety, chromatographic separation, and bioreactor operation as significant areas in which simulation methods can have a very important impact. These areas are being increasingly recognised as important components of modern chemical engineering.

Organisation of the Book

The book consists of an introduction to basic modelling presented in Chapters 1 through 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 Sec. 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 relationship between the model relationships described in the text and the resulting program remains 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 simulator's 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 distance.

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.

Some of our favourite examples from our previous books "Biological Reaction Engineering" and "Dynamics of Environmental Bioprocesses" have been added to this second edition in a new section of Chapter 5.

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.

Acknowledgements

We gladly acknowledge all who have worked previously in this field for the stimulation they have provided to us in the course of development of this book and our post-experience teaching. We are very fortunate in having the use of efficient PC and Macintosh based software, which was not available to those who were the major pioneers in the area of digital simulation. The modeller is now free to concentrate on the prime task of developing a realistic process model and to use this then in practical application, as was originally suggested by Franks (1967).

We are very grateful to all our past post-experience course participants and university students who have helped us to develop and improve some of the examples.

In addition, we would like to thank the following people at the Saarland University: Susan Lochow for help with the word processing and Patrick Cernko and Stefan Kiefer for converting most of the older ISIM programs to Madonna.

Finally, we are grateful to the developers of Berkeley Madonna for permission to include their software on our CD-ROM.

Nomenclature for Chapters 1 to 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	Dilution rate	1/s
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	Height	m
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	Constant	various
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
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	Slope of equilibrium line	–
m	Maintenance factor	kg substrate/ kg biomass s
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)	–
P	Products	–
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^3s
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_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

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
λ	Eigenvalues or root values	1/s
μ	Specific growth rate	1/s
μ_m	Maximum specific growth rate	1/s

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
d	Refers to death
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, mixer or measured
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
set	Refers to setpoint
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
$\bar{}$	Bar above symbol refers to dimensionless variable
'	Refers to perturbation variable, superficial velocity or stripping section
*	Refers to equilibrium concentration

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