

CHEMICAL REACTION ENGINEERING

THIRD EDITION

OCTAVE LEVENSPIEL

Chemical Reaction Engineering

Third Edition

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Preface

Chemical reaction engineering is that engineering activity concerned with the exploitation of chemical reactions on a commercial scale. Its goal is the successful design and operation of chemical reactors, and probably more than any other activity it sets chemical engineering apart as a distinct branch of the engineering profession.

In a typical situation the engineer is faced with a host of questions: what information is needed to attack a problem, how best to obtain it, and then how to select a reasonable design from the many available alternatives? The purpose of this book is to teach how to answer these questions reliably and wisely. To do this I emphasize qualitative arguments, simple design methods, graphical procedures, and frequent comparison of capabilities of the major reactor types. This approach should help develop a strong intuitive sense for good design which can then guide and reinforce the formal methods.

This is a teaching book; thus, simple ideas are treated first, and are then extended to the more complex. Also, emphasis is placed throughout on the development of a common design strategy for all systems, homogeneous and heterogeneous.

This is an introductory book. The pace is leisurely, and where needed, time is taken to consider why certain assumptions are made, to discuss why an alternative approach is not used, and to indicate the limitations of the treatment when applied to real situations. Although the mathematical level is not particularly difficult (elementary calculus and the linear first-order differential equation is all that is needed), this does not mean that the ideas and concepts being taught are particularly simple. To develop new ways of thinking and new intuitions is not easy.

Regarding this new edition: first of all I should say that in spirit it follows the earlier ones, and I try to keep things simple. In fact, I have removed material from here and there that I felt more properly belonged in advanced books. But I have added a number of new topics—biochemical systems, reactors with fluidized solids, gas/liquid reactors, and more on nonideal flow. The reason for this is my feeling that students should at least be introduced to these subjects so that they will have an idea of how to approach problems in these important areas.

I feel that problem-solving—the process of applying concepts to new situations—is essential to learning. Consequently this edition includes over 80 illustrative examples and over 400 problems (75% new) to help the student learn and understand the concepts being taught.

This new edition is divided into five parts. For the first undergraduate course, I would suggest covering Part 1 (go through Chapters 1 and 2 quickly—don't dawdle there), and if extra time is available, go on to whatever chapters in Parts 2 to 5 that are of interest. For me, these would be catalytic systems (just Chapter 18) and a bit on nonideal flow (Chapters 11 and 12).

For the graduate or second course the material in Parts 2 to 5 should be suitable.

Finally, I'd like to acknowledge Professors Keith Levien, Julio Ottino, and Richard Turton, and Dr. Amos Avidan, who have made useful and helpful comments. Also, my grateful thanks go to Pam Wegner and Peggy Blair, who typed and retyped—probably what seemed like *ad infinitum*—to get this manuscript ready for the publisher.

And to you, the reader, if you find errors—no, when you find errors—or sections of this book that are unclear, please let me know.

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Notation

Symbols and constants which are defined and used locally are not included here. SI units are given to show the dimensions of the symbols.

a	interfacial area per unit volume of tower (m^2/m^3), see Chapter 23
a	activity of a catalyst, see Eq. 21.4
a, b, \dots, r, s, \dots	stoichiometric coefficients for reacting substances A, B, ..., R, S, ...
A	cross sectional area of a reactor (m^2), see Chapter 20
A, B, ...	reactants
A, B, C, D,	Geldart classification of particles, see Chapter 20
C	concentration (mol/m^3)
C_M	Monod constant (mol/m^3), see Chapters 28-30; or Michaelis constant (mol/m^3), see Chapter 27
C_p	heat capacity ($\text{J}/\text{mol}\cdot\text{K}$)
C'_{pA}, C''_{pA}	mean specific heat of feed, and of completely converted product stream, per mole of key entering reactant ($\text{J}/\text{mol A} + \text{all else with it}$)
d	diameter (m)
d	order of deactivation, see Chapter 22
d^*	dimensionless particle diameter, see Eq. 20.1
D	axial dispersion coefficient for flowing fluid (m^2/s), see Chapter 13
\mathcal{D}	molecular diffusion coefficient (m^2/s)
\mathcal{D}_e	effective diffusion coefficient in porous structures ($\text{m}^3/\text{m solid}\cdot\text{s}$)
$\text{ei}(x)$	an exponential integral, see Table 16.1

E	enhancement factor for mass transfer with reaction, see Eq. 23.6
E	concentration of enzyme (mol or gm/m ³), see Chapter 27
E	dimensionless output to a pulse input, the exit age distribution function (s ⁻¹), see Chapter 11
E, E^*, E^{**}	RTD for convective flow, see Chapter 15
$E_{oo}, E_{oc}, E_{co}, E_{cc}$	RTD for the dispersion model, see Chapter 13
$Ei(x)$	an exponential integral, see Table 16.1
\mathcal{E}	effectiveness factor (-), see Chapter 18
f	fraction of solids (m ³ solid/m ³ vessel), see Chapter 20
f_i	volume fraction of phase i (-), see Chapter 22
F	feed rate (mol/s or kg/s)
F	dimensionless output to a step input (-), see Fig. 11.12
G_A	free energy (J/mol A)
h	heat transfer coefficient (W/m ² ·K), see Chapter 18
h	height of absorption column (m), see Chapter 24
H	height of fluidized reactor (m), see Chapter 20
H	phase distribution coefficient or Henry's law constant; for gas phase systems $H = p/C$ (Pa·m ³ /mol), see Chapter 23
H_A	mean enthalpy of the flowing stream per mole of A flowing (J/mol A + all else with it), see Chapter 9
H'_A, H''_A	enthalpy of unreacted feed stream, and of completely converted product stream, per mole of A (J/mol A + all else), see Chapter 19
ΔH_r	heat of reaction at temperature T for the stoichiometry as written (J)
$\Delta H_r, \Delta H_f, \Delta H_c$	heat or enthalpy change of reaction, of formation, and of combustion (J or J/mol)
k	reaction rate constant (mol/m ³) ¹⁻ⁿ s ⁻¹ , see Eq. 2.2
k, k', k'', k''', k''''	reaction rate constants based on r, r', r'', r''', r'''' , see Eqs. 18.14 to 18.18
k_d	rate constant for the deactivation of catalyst, see Chapter 21
k_{eff}	effective thermal conductivity (W/m·K), see Chapter 18
k_g	mass transfer coefficient of the gas film (mol/m ² ·Pa·s), see Eq. 23.2
k_l	mass transfer coefficient of the liquid film (m ³ liquid/m ² surface·s), see Eq. 23.3
K	equilibrium constant of a reaction for the stoichiometry as written (-), see Chapter 9

K_{bc}	bubble-cloud interchange coefficient in fluidized beds (s^{-1}), see Eq. 20.13
K_{ce}	cloud-emulsion interchange coefficient in fluidized beds (s^{-1}), see Eq. 20.14
L	characteristic size of a porous catalyst particle (m), see Eq. 18.13
L	half thickness of a flat plate particle (m), see Table 25.1
\dot{m}	mass flow rate (kg/s), see Eq. 11.6
M	mass (kg), see Chapter 11
n	order of reaction, see Eq. 2.2
N	number of equal-size mixed flow reactors in series, see Chapter 6
N_A	moles of component A
p_A	partial pressure of component A (Pa)
p_A^*	partial pressure of A in gas which would be in equilibrium with C_A in the liquid; hence $p_A^* = H_A C_A$ (Pa)
Q	heat duty ($J/s = W$)
r, r', r'', r''', r''''	rate of reaction, an intensive measure, see Eqs. 1.2 to 1.6
r_c	radius of unreacted core (m), see Chapter 25
R	radius of particle (m), see Chapter 25
R, S, \dots	products of reaction
R	ideal gas law constant, = 8.314 J/mol·K = 1.987 cal/mol·K = 0.08206 lit·atm/mol·K
R	recycle ratio, see Eq. 6.15
s	space velocity (s^{-1}); see Eqs. 5.7 and 5.8
S	surface (m^2)
t	time (s)
\bar{t}	= V/v , reactor holding time or mean residence time of fluid in a flow reactor (s), see Eq. 5.24
T	temperature (K or $^{\circ}C$)
u^*	dimensionless velocity, see Eq. 20.2
U	carrier or inert component in a phase, see Chapter 24
v	volumetric flow rate (m^3/s)
V	volume (m^3)
W	mass of solids in the reactor (kg)
X_A	fraction of A converted, the conversion (-)

X_A	moles A/moles inert in the liquid (-), see Chapter 24
Y_A	moles A/moles inert in the gas (-), see Chapter 24
Greek symbols	
α	m^3 wake/ m^3 bubble, see Eq. 20.9
δ	volume fraction of bubbles in a BFB
δ	Dirac delta function, an ideal pulse occurring at time $t = 0$ (s^{-1}), see Eq. 11.14
$\delta(t - t_0)$	Dirac delta function occurring at time t_0 (s^{-1})
ε_A	expansion factor, fractional volume change on complete conversion of A, see Eq. 3.64
ε	void fraction in a gas-solid system, see Chapter 20
\mathcal{E}	effectiveness factor, see Eq. 18.11
$\theta = t/\bar{t}$	dimensionless time units (-), see Eq. 11.5
K^m	overall reaction rate constant in BFB (m^3 solid/ m^3 gas·s), see Chapter 20
μ	viscosity of fluid ($kg/m\cdot s$)
μ	mean of a tracer output curve, (s), see Chapter 15
π	total pressure (Pa)
ρ	density or molar density (kg/m^3 or mol/m^3)
σ^2	variance of a tracer curve or distribution function (s^2), see Eq. 13.2
τ	$V/v = C_{A0}V/F_{A0}$, space-time (s), see Eqs. 5.6 and 5.8
τ	time for complete conversion of a reactant particle to product (s)
τ'	$= C_{A0}W/F_{A0}$, weight-time, ($kg\cdot s/m^3$), see Eq. 15.23
$\tau', \tau'', \tau''', \tau''''$	various measures of reactor performance, see Eqs. 18.42, 18.43
Φ	overall fractional yield, see Eq. 7.8
ϕ	sphericity, see Eq. 20.6
φ	instantaneous fractional yield, see Eq. 7.7
$\varphi(M/N) = \textcircled{M/N}$	instantaneous fractional yield of M with respect to N, or moles M formed/mol N formed or reacted away, see Chapter 7

Symbols and abbreviations

BFB	bubbling fluidized bed, see Chapter 20
BR	batch reactor, see Chapters 3 and 5
CFB	circulating fluidized bed, see Chapter 20
FF	fast fluidized bed, see Chapter 20

LFR	laminar flow reactor, see Chapter 15
MFR	mixed flow reactor, see Chapter 5
M-M	Michaelis Menten, see Chapter 27
$(M/N) = \varphi(M/N)$	see Eqs. 28.1 to 28.4
<i>mw</i>	molecular weight (kg/mol)
PC	pneumatic conveying, see Chapter 20
PCM	progressive conversion model, see Chapter 25
PFR	plug flow reactor, see Chapter 5
RTD	residence time distribution, see Chapter 11
SCM	shrinking-core model, see Chapter 25
TB	turbulent fluidized bed, see Chapter 20

Subscripts

<i>b</i>	batch
<i>b</i>	bubble phase of a fluidized bed
<i>c</i>	of combustion
<i>c</i>	cloud phase of a fluidized bed
<i>c</i>	at unreacted core
<i>d</i>	deactivation
<i>d</i>	deadwater, or stagnant fluid
<i>e</i>	emulsion phase of a fluidized bed
<i>e</i>	equilibrium conditions
<i>f</i>	leaving or final
<i>f</i>	of formation
<i>g</i>	of gas
<i>i</i>	entering
<i>l</i>	of liquid
<i>m</i>	mixed flow
<i>mf</i>	at minimum fluidizing conditions
<i>p</i>	plug flow
<i>r</i>	reactor or of reaction
<i>s</i>	solid or catalyst or surface conditions
0	entering or reference
θ	using dimensionless time units, see Chapter 11

Superscripts

a, b, . . .	order of reaction, see Eq. 2.2
<i>n</i>	order of reaction
o	refers to the standard state

**Dimensionless
groups**

$$\frac{D}{uL}$$

vessel dispersion number, see Chapter 13

$$\frac{D}{ud}$$

intensity of dispersion number, see Chapter 13

$$M_H$$

Hatta modulus, see Eq. 23.8 and/or Figure 23.4

$$M_T$$

Thiele modulus, see Eq. 18.23 or 18.26

$$M_w$$

Wagner-Weisz-Wheeler modulus, see Eq. 18.24 or 18.34

$$\text{Re} = \frac{du\rho}{\mu}$$

Reynolds number

$$\text{Sc} = \frac{\mu}{\rho D}$$

Schmidt number

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Chapter 1

Overview of Chemical Reaction Engineering

Every industrial chemical process is designed to produce economically a desired product from a variety of starting materials through a succession of treatment steps. Figure 1.1 shows a typical situation. The raw materials undergo a number of physical treatment steps to put them in the form in which they can be reacted chemically. Then they pass through the reactor. The products of the reaction must then undergo further physical treatment—separations, purifications, etc.—for the final desired product to be obtained.

Design of equipment for the physical treatment steps is studied in the unit operations. In this book we are concerned with the chemical treatment step of a process. Economically this may be an inconsequential unit, perhaps a simple mixing tank. Frequently, however, the chemical treatment step is the heart of the process, the thing that makes or breaks the process economically.

Design of the reactor is no routine matter, and many alternatives can be proposed for a process. In searching for the optimum it is not just the cost of the reactor that must be minimized. One design may have low reactor cost, but the materials leaving the unit may be such that their treatment requires a much higher cost than alternative designs. Hence, the economics of the overall process must be considered.

Reactor design uses information, knowledge, and experience from a variety of areas—thermodynamics, chemical kinetics, fluid mechanics, heat transfer, mass transfer, and economics. Chemical reaction engineering is the synthesis of all these factors with the aim of properly designing a chemical reactor.

To find what a reactor is able to do we need to know the kinetics, the contacting pattern and the performance equation. We show this schematically in Fig. 1.2.

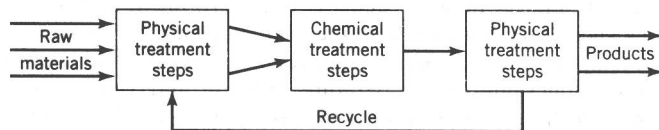


Figure 1.1 Typical chemical process.