CHEMICAL ENGINEERING MONOGRAPHS 13

Chemical Reactor Design in Practice

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To Jane

Preface

This text was compiled as a result of an invitation from Helsinki University of Technology to give a lecture course in "Practical Reactor Design", to follow on from their existing undergraduate introductory course as a senior course, also open to industrial participation.

There are a number of texts on reactor design now available, all of which cover the basic principles of the subject and discuss the present state of the art in various aspects of reactor engineering research. However, since reactor engineering research has moved from solving problems of practical interest to solving problems demanding high intellectual challenge, the available texts do not contain enough practical information to teach students how to design and specify reactors, or even to know the techniques by which this is done in technically advanced companies.

It is this void that this text is trying to fill.

In practice, reactor design usually starts by obtaining laboratory data from a new reaction system. It then sorts out the important factors, predicts a full-scale performance, and if this is attractive the pilot reactor is designed and operated. Data from the pilot reactor are then used in addition to laboratory data to design and predict the performance of a full-scale reactor that will work as optimally as possible, based on an economic criterion, and be easily operable and safe.

The engineer is best confronted with reactor problems at an early stage, when the chemist is going to look for good operating conditions, or even before, when he is thinking about the "reaction mechanism". The engineer can contribute to the search for optimum conditions, since he can bring economic factors into the picture and often has a numerate training which helps in the experimental planning and analysis of results.

The engineer produces a model from the laboratory results and uses this model for the design of his pilot and full-scale plant, for the choice of optimum conditions and for the stability analysis.

Reactor design in practice is concerned with the laboratory determination of data, their analysis, the development of models of the chemical and physical processes occurring, their optimization, the hardware dimensioning, and the definition of the necessary control and safety systems.

A text describing these activities touches on a multitude of disciplines - statistics, economics, optimization, control, and safety, as well as those subjects traditionally thought of as reactor design. This is an advantage for a senior course in that it is bringing together separate earlier courses, to show how, in practice, they are all needed to solve real problems.

The text was prepared for a 36 hours course plus nine two-hour exercise sessions. Since much of the course emphasized computer methods, the majority of the exercises were computer-based and run interactively with three or four students at each terminal. The nine exercises are included as Appendix 3, together with the programs used for the computer-based exercises.

The questions included at the end of each chapter are simply to emphasize the main point of that chapter and can be used by the reader to check that he has grasped the points that were being made.

It was the intention to compile a text of about 450 pages surveying the whole area of reactor design. When this is divided into topics and then further subdivided to produce a balanced text, it is surprising how few pages remain for the subjects that occupy volumes in the research literature because of the few recommendations that result from this activity. Whenever possible, only industrially tested techniques are described. When untried though promising methods are presented, a warning is given in the text. Since this is not a research text, no effort is made to substantiate the points made by reference to original literature. "Further Reading" lists are given where most points can be found discussed in more detail, and references are given only when the work would otherwise be difficult to find.

This "textbook" appears as a monograph because of the general feeling that not many teachers will be able to integrate this type of material into their present "reactor engineering" courses. If those teachers who do achieve this would contact the publishers, this would give some indication of the need for a textbook edition.

I would like to record my thanks to the staff of TKK Helsinki who made my stay in Finland so interesting and enjoyable - particularly to Professors B-son Bredenberg and Järveläinen, who arranged for the reactor design course to take place, and J. Aitamaa, who put much of his time into preparing the programs for the computer exercises.

Particular thanks are due to Elfriede Kilian for taking the major typing load and to Sirpa Pauni, who transferred some of my hand-written notes to typed text by a very novel, though somewhat laborious process.

Zürich, May 1981 L.M. Rose

Notation

a	empirical constant	-
a	interfacial area/unit volume	m^{-1}
A	cross-section area	m^2
A_i	pre-exponential factor (of reaction i)	$Kmol^{(1-n)} m^{3(n-1)} s^{-1}$
A'	heat-transfer area	m^2
b	empirical constant	-
c	empirical constant	-
c_i	cash flow for year i	$
c_p	mass specific heat at constant pressure	$kJ\ kg^{-1}\ K^{-1}$
C_A	molar concentration (of component A)	$kmol\ m^{-3}$
d (d_p, d_B, d_t, d_I, d_e)	diameter of particle, bubble, tube, impeller or equivalent diameter	m
D	reactor diameter	m
D_A	molecular diffusivity (of component A)	$m^2\ s^{-1}$
E_i	activation energy (of reaction i)	$kJ\ kmol^{-1}$
E'	enhancement factor	-
f	fanning friction factor	-
f	fraction capital costs incurred annually	-
F	molar flowrate	$kmol\ s^{-1}$
F	objective function	-
F'	tax factor	-
g	gravitational constant	$9.81\ m\ s^{-2}$
g_g	heat generation/unit reactor volume	$kJ\ m^{-3}$
g_r	heat removed/unit reactor volume	$kJ\ m^{-3}$
G	mass flowrate (gas)	$kg\ s^{-1}$
G	free energy	$kJ\ kmol^{-1}$
h	single film heat-transfer coefficient	$kW\ m^{-2}\ K^{-1}$
H	enthalpy	$kJ\ kmol^{-1}$
H'	Henry's law solubility constant	$bar\ m^3\ kmol^{-1}$
ΔH_i	heat of reaction (of i^{th} reaction)	$kJ\ kmol^{-1}$
I	investment cost	$
k_i	reaction rate constant (of i^{th} reaction)	$kmol^{(1-n)}\ m^{3(n-1)}\ s^{-1}$
k_g	gas film mass-transfer coefficient	$kmol\ m^{-2} bar^{-1}\ s^{-1}$
k_L	liquid film mass-transfer coefficient	$m\ s^{-1}$
K (K_a, K_c)	equilibrium constant (based on activity, concentration)	-
K_g	overall gas mass-transfer coefficient	$kmol\ m^{-2}\ bar^{-1}\ s^{-1}$

K_A	absorption coefficient	bar^{-1}
K', K", K'''	miscellaneous constants	-
L	length	m
$L_{\frac{1}{2}}$	catalyst life (number of half lives)	-
L	project life	years
L'	mass flowrate (liquid)	$kg\ s^{-1}$
m	lifetime for taxation purposes	years
M_A	molecular weight (of A)	$kg\ kmol^{-1}$
n_A	number of kmoles (of A)	kmol
$\dot{n}_A$	molar flowrate (of A)	$kmol\ s^{-1}$
N	stirrer speed (RPS)	s^{-1}
N	number of tubes, number of beds, number of tanks	-
N_{C_a}	dimensionless group in Calderbank's surface area equations	-
N_P	agitator power number	-
N_{Re}	Reynolds number	-
p_A	partial pressure (of A)	bar
P	total pressure	bar
P', P'_g	agitator power (ungassed and gassed)	kW
P"	power supplied by gas	kW
Q	volumetric flowrate	$m^3\ s^{-1}$
r	fractional rate of interest	-
r	recycle rate	$kmol\ s^{-1}$
r_i	molar reaction rate/unit reactor volume	$kmol\ m^{-3}\ s^{-1}$
r_t	fractional taxation rate	-
R	gas constant	$8.314\ kJ\ kmol^{-1}\ K^{-1}$ or $0.08314\ bar\ m^3\ kmol^{-1}\ K^{-1}$
s	tube pitch	m
s'	stirrer tip speed	$m\ s^{-1}$
S	entropy	$kJ\ K^{-1}\ kmol^{-1}$
S	selectivity	-
t	time	s
$t_{\frac{1}{2}}$	half-life time	s
t_F	residence time in the film	s
t_R	residence time of the reaction	s
$\bar{t}$	mean residence time of a distribution	s
T	temperature	K
T'	production	$kmol\ s^{-1}$ or tons $year^{-1}$
u	velocity	$m\ s^{-1}$
u_s, u_t, u_m	superficial, terminal, minimal velocity	$m\ s^{-1}$

U	overall heat-transfer coefficient	kW m^{-2} K^{-1}
V	volume	m^3
V_R	reactor volume	m^3
w	width	m
W	weight	tons
x	independent variable	-
x_A	mole fraction in liquid (of A)	-
X_A	fractional conversion (of A)	-
y	dependent variable	-
y_A	mole fraction in gas (of A)	-
Z	film thickness	m

GREEK LETTERS

α	empirical constant	-
ε_g	gas hold up in gas/liquid dispersions	-
ε_p	void fraction in packed bed	-
λ	thermal conductivity	kW m^{-1} K^{-1}
θ	reduced time	-
μ	dynamic viscosity	kg m^{-1} s^{-1}
ν	stoichiometric coefficient (-ve for reactants)	-
σ	surface tension	kg s^{-2}
π	3.1416	-
ρ	mass density	kg m^{-3}
τ	space time	s
η	effectiveness factor (gas/solid reactions)	-
β	pellet temperature rise factor	-
ϕ	Thiele modulus	-

SUBSCRIPTS

A, B ...	for components A, B ...
amb	ambient conditions
b	in bulk (fluid)
g	in gas phase (or in presence of gas)
i	for ith reaction
in	of inlet
j	for jth species
J	of jacket
L	in liquid phase
0	at initial (or reference) condition

out	of outlet
R	of reactor
s	at solid surface, of solid
S	for standard case
U	for utilities
w	at wall

GENERAL NOTE ON UNITS

SI units have been used throughout, but in order to be able to deal with conveniently sized numbers the following have been consistently used: m, kg, kmol, kJ, kW, s, K, bar.

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