

Experiments in Catalytic  
Reaction Engineering

0056397

Studies in Surface Science and Catalysis

Advisory Editors: B. Delmon and J.T. Yates

Vol. 124

# EXPERIMENTS IN CATALYTIC REACTION ENGINEERING

by

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1999

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Amsterdam — Lausanne — New York — Oxford — Shannon — Singapore — Tokyo

ELSEVIER SCIENCE B.V.  
Sara Burgerhartstraat 25  
P.O. Box 211, 1000 AE Amsterdam, The Netherlands

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First edition 1999

#### Library of Congress Cataloging-in-Publication Data

Berty, J. M. (Jozsef M.)

Experiments in catalytic reaction engineering / by J.M. Berty. --  
1st ed.

p. cm. -- (Studies in surface science and catalysis ; 124)

Includes bibliographical references and index.

ISBN 0-444-82823-0 (alk. paper)

1. Catalysis. 2. Chemical reactors. I. Title. II. Series.

TP156.C35B47 1999

660'.2995--dc21

99-35157

CIP

ISBN: 0 444 82823 0

Ⓢ The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).  
Printed in The Netherlands.

## Preface

Many present day technologies were developed on an empirical basis, through much hard work and with remarkable success. However, all were achieved without benefit of a basic understanding of rate controlling processes, and the interaction of transport processes with chemical kinetics. These interactions are most important with fast reactions that are strongly exothermic or endothermic, exactly the ones preferred for industrial production. Therefore, many opportunities exist for improving present day production technologies through a better insight into the details of rate processes.

The influence of transport process in two-phase reaction systems depends on flow conditions, which change with the size of the equipment. This is the reason for the historic observation that performance changes as processes are scaled up and therefore scale-up should be done in several steps, each limited to a small increase in size. This is a slow and expensive method and still does not guarantee optimum design.

Effects of transport processes cannot be ignored in investigations aimed at more fundamental aspects of kinetics and catalysis. The interaction of chemical and physical processes was noticed a long time ago. M. V. Lomonosov mentioned in 1745:

“I not only saw from other authors, but am convinced by my own art, that chemical experiments combined with physical, show peculiar effects.”<sup>1</sup>

The need to design production units on a fundamental kinetic basis was recognized for a long time, yet the basic need to distinguish between rates influenced by transport and true chemical rates, was not fully comprehended and came only later.

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<sup>1</sup> As quoted by Frank-Kamenetskii (1961) in the preface to his book.

At the First European Symposium on Chemical Engineering, Amsterdam, (1957) the definition for Chemical Reaction Engineering was accepted as:

“Chemical reaction engineering is part of chemical engineering in general. It aims at controlling the chemical conversion on a technical scale and will ultimately lead to appropriate and successful reactor design. An important part is played by various factors, such as flow phenomena, mass and heat transfer, and reaction kinetics. It will be clear that in the first place it is necessary to know these factors separately.

Yet this knowledge in itself is insufficient. *The development of chemical conversion on a technical scale can only be understood from the relation and interaction between the above mentioned factors*”.

Damköhler (1936) studied the above subjects with the help of dimensional analysis. He concluded from the differential equations, describing chemical reactions in a flow system, that four dimensionless numbers can be derived as criteria for similarity. These four and the Reynolds number are needed to characterize reacting flow systems. He realized that scale-up on this basis can only be achieved by giving up complete similarity. The recognition that these basic dimensionless numbers have general and wider applicability came only in the 1960s. The Damköhler numbers will be used for the basis of discussion of the subject presented here as follows:

$$Da_I = \frac{rl}{Cu}, \quad Da_{II} = \frac{rl^2}{CD}, \quad Da_{III} = \frac{r(-\Delta H_r)l}{c_p \rho T u},$$

$$Da_{IV} = \frac{r(-\Delta H_r)l^2}{k_t T}, \quad Re = \frac{l u \rho}{\mu}.$$

In a later paper Damköhler (1937) also defined :

$$Da_v = Da_{IV}/Nu = \frac{r(-\Delta H_r)l}{hT}$$

This will be used here, too.

In the mid 1960s, computers became available and this made many calculations possible, including the simultaneous integration of several coupled differential equations. With this, the execution of many design

tasks—formerly very time consuming and approximate—became easy, fast and seemingly accurate. Publications proliferated, with computer solutions to many imagined and a few real problems. Only then was it realized that good kinetic results, free of transfer influences, were woefully lacking. This caused a general increase of interest in improving kinetic measurements.

In 1960 the author was charged with the review and improvement of the ethylene oxide technology of Union Carbide Corporation (UCC). A historic overview revealed some interesting facts. The basic French patent of Lefort (1931,1935) for ethylene oxide production was purchased by UCC in 1936. In 1937, a pilot-plant was operated and commercial production started in 1938. By 1960, UCC's production experience was several hundred reactor-years. This was expressed as the sum of the number of production reactors, each multiplied by the number of years it had been in operation. Research and development had continued since the purchase of the original patent and the total number of people involved in ethylene oxide related research at one time reached one hundred.

Development of the first recycle reactor was one of the consequences of a challenging situation. The ethylene oxide process had reached a high level of sophistication and excellent performance after 25 years of continuous R&D. To improve results achieved by so many excellent people over so many years was a formidable task.

In previous studies, the main tool for process improvement was the tubular reactor. This small version of an industrial reactor tube had to be operated at less severe conditions than the industrial-size reactor. Even then, isothermal conditions could never be achieved and kinetic interpretation was ambiguous. Obviously, better tools and techniques were needed for every part of the project. In particular, a better experimental reactor had to be developed that could produce more precise results at well defined conditions. By that time many home-built recycle reactors (RRs), spinning basket reactors and other laboratory continuous stirred tank reactors (CSTRs) were in use and the subject of publications. Most of these served the original author and his reaction well but few could generate the mass velocities used in actual production units.

Recycle reactors at that time were called "Backmix Reactors." They were correctly considered the worst choice for the production of a reactive intermediate, yet the best for kinetic studies. The aim of the kinetic study for ethylene oxidation was to maximize the quality of the information, leaving the optimization of production units for a later stage in engineering studies. The recycle reactors could provide the most precise results at well defined conditions even if at somewhat low selectivity to the desired product.

The RR developed by the author at UCC was the only one that had a high recycle rate with a reasonably known internal flow (Berty, 1969). This original reactor was named later after the author as the "Berty Reactor". Over five hundred of these have been in use around the world over the last 30 years. The use of Berty reactors for ethylene oxide process improvement alone has resulted in 300 million pounds per year increase in production, without addition of new facilities (Mason, 1966). Similar improvements are possible with many other catalytic processes. In recent years a new blower design, a labyrinth seal between the blower and catalyst basket, and a better drive resulted in an even better reactor that has the registered trade name of "ROTOBERTY®."

Many of the methods discussed in this book stem from the practical experience of the author, who worked for 20 years at Union Carbide Corporation. Other experience came from consulting work for over 30 companies, and from the laboratory of Berty Reaction Engineers, Ltd. The corresponding theoretical treatments were developed while teaching six professional short courses and lecturing at the State University of New York at Buffalo, NY, The University of Akron, at Akron, OH, and as a Senior Fulbright Scholar at the Technical University of Munich, Germany. The final assembly of the book was started when the author again taught a short course at the University of Veszprém in Hungary after a 36 year interruption.

The aim of the book is to give practical advice for those who want to generate kinetic results, valid for scale-up, and backed by sensible theory and understandable mathematical explanation.

Methanol synthesis will be used many times as an example to explain some concepts, largely because the stoichiometry of methanol synthesis is simple. The physical properties of all compounds are well known, details of many competing technologies have been published and methanol is an important industrial chemical. In addition to its relative simplicity, methanol synthesis offers an opportunity to show how to handle reversible reactions, the change in mole numbers, removal of reaction heat, and other engineering problems.

To facilitate the use of methanol synthesis in examples, the “UCKRON” and “VEKRON” test problems (Berty et al 1989, Árva and Szeifert 1989) will be applied. In the development of the test problem, methanol synthesis served as an example. The physical properties, thermodynamic conditions, technology and average rate of reaction were taken from the literature of methanol synthesis. For the kinetics, however, an artificial mechanism was created that had a known and rigorous mathematical solution. It was fundamentally important to create a fixed basis of comparison with various approximate mathematical models for kinetics. These were derived by simulated experiments from the test problems with added random error. See Appendix A and B, Berty et al, 1989.

The “UCKRON” AND “VEKRON” kinetics are not models for methanol synthesis. These test problems represent assumed four and six elementary step mechanisms, which are thermodynamically consistent and for which the rate expression could be expressed by rigorous analytical solution and without the assumption of rate limiting steps. The exact solution was more important for the test problems in engineering, than it was to match the presently preferred theory on mechanism.

Conclusions from the test problems are not limited by any means to methanol synthesis. These results have more general meaning. Other reactions also will be used to explain certain features of the subjects. Yet the programs for the test problem make it possible to simulate experiments on a computer. In turn, computer simulation of experiments by the reader makes the understanding of the experimental concepts in this book more profound and at the same time easier to grasp.

The author wants to express his most sincere gratitude to all his colleagues, coworkers and students who participated in the work leading to this book. Their names are listed in the cited publications of the author. Thanks are due for proofreading the original manuscript to Mr. Imre J. Berty, P. E.. For reviewing this book and editing it for publication, special thanks are due to Ms. Gail B. C. Marsella of Branch Text Press.

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**Notations**

Symbol	Definition	Units
$A_i$	chemical compound	mol
$a$	thermal diffusivity = $k_t / c_p$	$m^2/s$
$a_i$	activity = $(f/f_o)$	–
$C_i$	concentration of species $A_i$	$mol/m^3$
$c$	specific heat of fluid	$kJ / kg K$
$D_{AB}$	diffusivity of A in B	$m^2/s$
$d_p$	particle diameter	m
$d_t$	tube diameter, inside	m
$E$	energy of activation	$kJ/kmol$
$F$	force = newton	$kg m/s^2$
$F$	total molar flow rate	$mol / s$
$F_i$	molar flow rate of $A_i$	$mol / s$
$F'$	volumetric flow rate	$m^3/s$
$f$	fugacity = pascal	Pa
$G$	mass velocity	$kg / m^2 s$
$g$	acceleration of gravity = 9.81	$m^2/s$
$\Delta H$	heat of reaction	$kJ / mol$
$h_f$	film coefficient for heat transfer	$W / m^2 s$
$K$	equilibrium constant = $a_p^P / a_R^r$	–
$k$	reaction rate coefficient	$l / s$
$k_x$	mass transfer coefficient	$m / s$
$k_t$	thermal conductivity	$W / m K$
$k_m$	momentum transfer coefficient	$m / s$
$l$	distance	m
$M$	molar density, $l/1000 MW$	$mol/kg$
$m$	integral number	–
$MW$	molecular weight	$kg / kmol$
$N$	number of moles	mol
$n$	order of reaction	–
$P$	pressure	kPa
$R$	gas constant = 8.314	$J/mol K$
$R_i$	total rate of change of $A_i$	$mol / m^3 s$
$R_t$	inside tube radius	m
$r_i$	rate of reaction $i$	$mol / m^3 s$
$q_{gen}$	rate of heat generation	$W/m^3$
$S$	selectivity, fractional	–
$S$	surface	$m^2$
$SS$	steady state	–
$T$	temperature	K

Symbol	Definition	Units
t	clock time	s
u	linear velocity	m / s
U	overall heat transfer coefficient	W / m <sup>2</sup> K
U <sub>0</sub>	time constant ratio	–
V	volume	m <sup>3</sup>
W	weight of catalyst	kg
w	power = watts	W
x	mole fraction in liquid, on catalyst surface	–
X	conversion, fractional	–
y	mol fraction in gas	–
Y	Yield, fractional	–
Z	Efficiency, fractional	–

### Greek Letters

$\alpha$	stoichiometric coefficient	–
$\beta$	adiabatic temperature rise potential	–
$\gamma$	Arrhenius number = $E / RT^2$	–
$\delta$	change in the sum of stoichiom. no.s	–
$\varepsilon$	void fraction in catalyst bed	–
$\eta$	kinematic viscosity	m <sup>2</sup> / s
$\eta$	catalytic effectiveness factor, fractional	–
$\theta$	void fraction in catalyst pores	–
$\mu$	dynamic viscosity	kg / m s
$\rho$	density	kg / m <sup>3</sup>
$\tau$	tortuosity factor	–
$\phi$	Thiele modulus = $(d_p/3)(k/D)^{0.5}$	–
$\Theta$	Weisz–Prater criterion = $\eta h \phi^2 = Da_{II}$	–

### Superscripts

s at standard temp and press. of 273.1 K and 101.3 kPa

**Subscripts**

b	bed	
f	fluid	–
i	reactions	–
j	compounds	
m	mass	–
o	feed conditions	–
p	particle	–
P	products	–
R	reactants	–
C	catalyst	
S	surface	–
s	solid	–
t	total	–

**Dimensionless Numbers**

'A'	momentum transfer / momentum cond., (analog to Sh and Nu numbers)	$= k_m l / \eta$
'B'	momentum production/momentum cond., (analog to St and $f' / 2$ numbers)	$= F / \rho \eta u l$
Bi	Biot (heat transfer/thermal cond. of solid)	$= Nu(k_r/k_{t,s})$
Bo	Bodenstein (Pe number for mass)	$= u l / D$
$\beta$	adiabatic temperature rise potential	$= C(-\Delta H) / \rho c T$
Ca	Carberry	$= r l / C k_m$
$Da_I$	Damköhler number – I	$= r l / C u$
$Da_{II}$	Damköhler number – II	$= r l^2 / C D$
$Da_{III}$	Damköhler number – III	$= r (-\Delta H) l / \rho c T u$
$Da_{IV}$	Damköhler number – IV	$= r (-\Delta H) l^2 / k_t$
$Da_V$	Damköhler number – V	$= r (-\Delta H) l / h T$
$f / 2$	Fanning friction factor	$= k_m / u$
'E'	momentum production/ conduction	$= F / \rho k_m u l^2$
Fr	Froud = $1/Fa = 1/\text{Fanning}$	$= u^2 / g l$
Ha	Hatta number	$= \sqrt{(kD)/k_g}$
$j_D$	Colburn factor for mass ( $Sh Sc^{2/3}$ )	$= (k_g l / D)(\eta/D)^{0.66}$
$j_H$	Colburn factor for heat ( $St Pr^{2/3}$ )	$= (h / \rho c u)(\eta/a)^{0.66}$
Le	Lewis number	$= a / D$
Nu	Nusselt number	$= h l / k_t$
Pe	Peclet number	$= u l / a$
Pr	Prandtl number	$= \eta / a = c\mu/k_t$

Re	Reynolds number	$= u l / \eta$
Sc	Schmidt number	$= \eta / D$
Sh	Sherwood number	$= k_g l / D$
St	Stanton number	$= h / \rho c u$
St'	Stanton number for mass	$= k_g / u$
We	Weber number	$= \rho u^2 l^2 / F$

**A, B, E** are unnamed numbers results of the systematization by László (1964).

The unnamed number **C** is now called the Carberry number, and **D** is identical with  $\mathbf{Da}_{IV} = \mathbf{Da}_V$ .

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