

## CHEMICAL REACTOR ENGINEERING\*

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**T**HE DEVELOPMENT OF chemical reaction engineering as an identifiable area within chemical engineering has led to renewed interest and emphasis on courses dealing with chemical reaction kinetics and chemical reactor design. The basic issues concerning instruction in these areas are probably not much different from those involved in any other area of chemical engineering insofar as fundamentals vs. applications, extent of coverage, and similar factors. There is, however, a chemical factor involved in this area that may not appear quite so prominently in other endeavors, and instruction at the undergraduate level particularly may be sensitive to the contents of current offerings in chemistry courses.

Certainly there is no lack of literature on all aspects of the topic. In Table 1 is given an extensive (but by no means comprehensive) list of references dealing with chemical kinetics, engineering aspects of kinetics and reactor design, experimental methods, catalysis, and several specialized topics. Most of us are possibly familiar with the offerings listed under engineering aspects, and a quick glance at this tabulation might induce one to think there is an enormous variation in what individuals conceive to be useful components of an undergraduate course. It is interesting to see if this is really so. Let us do this by comparing the table of contents of three typical offerings from the list, as shown in Table 2. Two of the books, by Smith and Levenspiel, were chosen because they are perhaps the most widely used undergraduate texts. The third book, by Carberry, is a very recent addition to the kinetic literature. In each case the author has chosen to treat a number of funda-

mental topics, with more specialized applications in later chapters. Descriptive kinetics and data interpretation are, logically, accorded first place on each list, followed by introductory material on reactor design and analysis. The latter is largely limited to ideal reactor models; the effect of temperature is treated somewhat differently in an organizational manner by the three authors, but the level and extent of coverage is quite similar. Concepts of selectivity as well as rate and conversion are presented early in each case and maintained as an important factor in kinetics and reactor analysis throughout. Following this introductory material, each author then turns to problems associated with deviations from ideal reactor performance. Here somewhat more variation is apparent in organization and presentation but, again, the net coverage and information is quite similar.

The point is that, in terms of information which might form the core content of a typical



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**Gene Petersen** did his undergraduate and masters work at the University of Washington and obtained his Ph.D. in Fuel Science at Pennsylvania State University in 1953. He joined the faculty at the University of California at Berkeley where he pursues research and teaches kinetics, catalysis and reaction engineering. (R)

\*ASEE Summer School for ChE Faculty, Snowmass Resort, Colorado, August, 1977.

**TABLE 1.**  
**Selected References in Chemical Kinetics,**  
**Catalysis and Reactor Design**

**Basic Material For Review:**

- E. L. King, "How Chemical Reactions Occur", Benjamin, 1964 (Paperback).
- F. Daniels and R. A. Alberty, "Physical Chemistry", Wiley.
- Latham, J. L., "Elementary Reaction Kinetics", 2nd ed., Butterworths (1969).

**Introductory Texts Emphasizing Chemical Aspects Of Subject:**

- A. A. Frost and R. G. Pearson, "Kinetics and Mechanism", 2nd ed., Wiley, 1969.
- K. J. Laidler, "Chemical Kinetics", 2nd ed., McGraw-Hill, 1965.
- K. J. Laidler, "Reaction Kinetics", Volumes I and II, Pergamon Press, 1963 (Paperback).
- C. N. Hinshelwood, "Kinetics of Chemical Change", Clarendon Press, 1940 (Somewhat out of date, but contains a good qualitative discussion of basics).
- M. Boudart, "Kinetics of Chemical Processes", Prentice-Hall, 1968.
- I. Amdur and G. G. Hammes, "Chemical Kinetics", McGraw-Hill, 1966.

**More Advanced Treatments:**

- H. S. Johnston, "Gas Phase Reactions", Prentice-Hall.
- N. Semenov, "Some Problems in Chemical Kinetics and Reactivity", Vol. I and II, trans. by M. Boudart, Princeton Univ. Press, 1958, 1959.
- S. W. Benson, "Foundations of Chemical Kinetics", McGraw-Hill, 1960.
- V. N. Kondratiev, "Kinetics of Chemical Gas Reactions", 1958, trans. from the Russian, Pergamon Press, 1964.
- S. Glasstone, K. J. Laidler and H. Eyring, "The Theory of Rate Processes", McGraw-Hill, 1941.

**Texts Emphasizing Engineering Aspects of Kinetics and Reactor Design:**

- O. Levenspiel, "Chemical Reaction Engineering", 2nd ed., Wiley, 1972.
- J. M. Smith, "Chemical Engineering Kinetics", McGraw-Hill, 2nd ed., 1970.
- S. M. Walas, "Reaction Kinetics for Chemical Engineers", McGraw-Hill, 1959.
- O. A. Hougen and K. M. Watson, "Chemical Process Principles", Vol. III, Wiley, 1947.
- R. Aris, "Introduction to the Analysis of Chemical Reactors", Prentice-Hall, 1965.
- K. G. Denbigh, "Chemical Reactor Theory", Cambridge Univ. Press, 1966.
- H. Kramers and K. R. Westerterp, "Elements of Chemical Reactor Design and Operation", Academic Press, 1963.
- D. A. Frank-Kamenetskii, "Diffusion and Heat Exchange in Chemical Kinetics", Trans. Ed. John P. Appleton, 2nd ed., Plenum Press, 1969.
- G. R. Gavalas, "Nonlinear Differential Equations of Chemical Reacting Systems", Springer-Verlag, 1968.
- J. J. Carberry, "Chemical and Catalytic Reaction Engineering", McGraw-Hill, 1976.

L. C. Lee and W. J. Thomas, "Chemical Engineering", Vol. III, edited by J. F. Richardson and D. G. Peacock, Chapters 1 and 2, Pergamon, 1971.

C. G. Hill, Jr., "Chemical Engineering Kinetics and Reactor Design", Wiley, 1977.

**Experimental Techniques:**

- H. W. Melville and B. G. Gowenlock, "Experimental Methods in Gas Reactions", Macmillan, 1964.
- S. L. Friess and A. Weissberger (Editors), "Investigations of Rates and Mechanisms of Reactions", Volumes I and II (Volume 8, parts 1 and 2, of "Technique of Organic Chemistry"), Interscience, 1953 and 1963.
- R. Anderson, "Experimental Methods in Catalytic Research", Academic Press, 1968. Volumes I, II, and III.

**Heterogeneous Catalysis:**

- J. M. Thomas and W. J. Thomas, "Introduction to the Principles of Heterogeneous Catalysis", Academic Press, 1967.
- E. E. Petersen, "Chemical Reaction Analysis", Prentice-Hall, 1965.
- P. G. Ashmore, "Catalysis and Inhibition of Chemical Reactions", Butterworths, 1963.
- J. R. Anderson, "Structure of Metallic Catalysts", Academic Press, 1975.
- R. Aris, "The Mathematical Theory of Diffusion and Reaction in Permeable Catalysts", Volumes I and II, Oxford, 1975.
- C. N. Satterfield, "Mass Transfer in Heterogeneous Catalysis", MIT Press, 1970.
- G. C. Bond, "Heterogeneous Catalysis", Clarendon Press, 1974.
- G. C. Szabo (Editor), "Contact Catalysis", Elsevier, 1976, Volumes I and II.

**Special Topics:**

- J. Szekeley, J. W. Evans and H. Y. Sohn, "Gas Solid Reactions", Academic Press, 1976.
- D. Kunii and O. Levenspiel, "Fluidization Engineering", Wiley, 1969.
- D. F. Othmer, "Fluidization", Reinhold, 1956.

undergraduate course, there is considerable agreement on content and even order of presentation. This is not to say that these texts, or others, are all the same, for in the latter stages of each there appears considerable variation in content and organization, indicative of individual interests and perhaps specialized applications. The manner of presentation varies considerably to reflect the style of the author. This is shown in Table 3 which presents the content of the basic undergraduate courses at Berkeley and Northwestern. This diversity leads to what we believe to be a healthy variation in individual undergraduate courses around the country, in which the fundamentals are fairly well agreed upon but many different approaches exist within presentation and the use of

**TABLE 2.**  
**Tables of Contents of Basic Material from Three Texts on**  
**Chemical Engineering Kinetics and Reactor Design**

| Levenspiel  |            | Smith  |                     | Carberry  |            |
|---|------------|--|---------------------|---|------------|
| 1. Introduction   | 7          | 1. Introduction  | 32                  | 1. Introduction                                   | 11         |
| 2. Kinetics of Homogeneous Reactions                          | 33         | 2. Kinetics of Homogeneous Reactions   | 65                  | 2. Behavior of Chemical Reactions                 | 50         |
| 3. Interpretation of Batch Reactor Data                       | 52         | 3. Design Fundamentals   | 33                  | 3. Behavior of Chemical Reactors                  | 66         |
| 4. Introduction to Reactor Design                             | 4          | 4. Homogeneous Reactor Design: Isothermal Conditions                             | 73                  | 4. Conservation Equations for Reactors            | 51         |
| 5. Single Ideal Reactors                                      | 27         | 5. Temp. Effects in Homogeneous Reactors   | 40                  | 5. Heterogeneous Reactions                        | 50         |
| 6. Design for Single Reactions                                | 39         | 6. Deviations from Ideal Reactor Performance                                     | 30                  | 6. Gas-Liquid and Liquid-Liquid Systems           | 67         |
| 7. Design for Multiple Reactions                              | 47         | 7. Heterogeneous Reactions   | 9                   | 7. Fluid-Solid Non-Catalytic Reactions            | 47         |
| 8. Temp. and Pressure Effect                                  | 43         | 8. Heterogeneous Catalysis   | 47                  | 8. Heterogeneous Catalysis and Catalytic Kinetics | 100        |
| 9. Non-Ideal Flow   |            | 9. Kinetics of Fluid-Solid Catalytic Reactions                                   | 28                  |   |            |
| 10. Mixing of Fluids  |            | 10. External Transport Processes in Heterogeneous Reactions                      | 42                  |   |            |
| 11. Introduction to Design for Heterogeneous Reacting Systems | 8          | 11. Reaction and Diffusion Within Porous Catalysts: Internal Transport Processes | 65                  |   |            |
| 14. Solid Catalyzed Reactions                                 | 77         |  |                     |   |            |
| <b>Total pages:</b>   | <b>337</b> |  |                     | <b>Total pages:</b>                               | <b>442</b> |
|   |            |  | <b>Total pages:</b> |   |            |
|   |            |  | <b>464</b>          |   |            |

specific examples to develop material beyond the entry level. Historically this situation may be the result of the fact that many current undergraduate courses in reaction kinetics and reactor analysis had their origins not too long ago at the graduate level. It is within recent memory that many undergraduate curricula contained no courses (or elective, at best) in this area.

#### KINETICS AND EXPERIMENTATION

**T**HERE ARE SOME ASPECTS of undergraduate education concerning kinetics and reaction engineering that should be of current concern. Interestingly, most of them deal with kinetics. One has to do with the chemical part of chemical kinetics. In most cases this is not treated in any detail, if at all, with the result that the student's analysis of kinetics is based purely on phenomono-

logical rate laws with little understanding of their basis. Where does the Arrhenius law come from anyway? If we are careful to use activities in thermodynamic problems, shouldn't we use them in kinetics? Certainly all of us could formulate numerous questions similar to these and perhaps even admit that they are not addressed in our undergraduate course. Earlier, such problems may not have been of quite so much concern, but current undergraduate physical chemistry courses differ from those taught 20 years ago. Increased emphasis (if not total preoccupation) on spectroscopy and quantum theory has reshaped much of the course content and the student may come away with somewhat less chemical intuition regarding reaction analysis than was formerly the case.\* A problem in developing suitable coverage is that text material is distributed over a wide range of sources, as indicated in Table 1.

A second factor of concern is the development of suitable laboratory experiments in the area. Too often relevant experimentation is found only as one or two entrees in the undergraduate chem-

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\*Do you know what your Chemistry Department is doing tonight?

ical engineering laboratory menu, or an occasional experiment in introductory or physical chemistry laboratory. This is admittedly a difficult problem, since the timing sequence of courses in kinetics in many curricula does not make for convenient relation between classroom and laboratory experience. Unfortunately we have no general solutions to set forth for this problem, but we feel strongly that the undergraduate program in kinetics should not be devoid of relevant experimentation in an engineering context. In fact, experiments on non-trivial catalytic, kinetic and reactor design systems introduce the student to the real world and focus attention on the enormous difficulties associated with getting good data, interpreting them, and using them to predict reactor behavior. An undergraduate elective course, half lecture and half laboratory, is available at Berkeley. The course outline is shown in Table 4. A course with a similar objective was developed some years ago at Princeton and a laboratory manual detailing several excellent experiments was prepared by J. B. Anderson.

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### ENTRANCE-LEVEL COURSES

IT IS INTERESTING that an increasing number of schools throughout the country are offering two courses in this area at the undergraduate level, either as a Junior-Senior sequence or by making available the entering level graduate course as a second offering for qualified undergraduates. This, in turn, presents an interesting problem as to what to offer students entering a graduate program with such a background. Probably, any graduate program should include at least one course beyond the entering level, and many do considerably more. Often the advanced graduate

**TABLE 3.**  
**Undergraduate Kinetic Courses Compared**

| Northwestern University<br>4 hr/wk of lecture for 10 weeks |  | California, Berkeley<br>3 hr/wk lecture and 1 hr tutorial for 10 wks |  |
|--|--|--|--|
| Week   | Content  | Week   | Content  |
| 1  | Introduction, definition of rate and extent of reaction<br>Descriptive kinetics of simple and nearly complex reactions<br>Elementary steps and chain reactions           | 1  | Introduction to subject, references, purpose, relationship to other chemical engineering courses<br>Stoichiometric equations, simple and complex reactions<br>Extent of reaction, rate of reaction<br>Elementary steps, sequences of reactions |
| 2  | Nonisothermal reactions<br>Interpretation of kinetic data  | 2  | Temperature coefficient, Arrhenius expression<br>Theories of reaction—collision theory and transition state theory   |
| 3  | Collision theory, Lindemann theory   | 3  | Finish transition state theory<br>Steady state approximation   |
| 4  | Midterm I (basic kinetics)<br>RRK theory, transition state theory  | 4  | Rate limiting step—meaning and utility<br>Examples of homogeneous and heterogeneous systems. HBr, HI, dehydrogenation of methylcyclohexane   |
| 5  | Reactions on surfaces<br>Mixing and segregation<br>Age distributions   | 5  | Plug flow reactor isothermal, adiabatic and non-isothermal   |
| 6  | Midterm II (rate theories)<br>Mixing models  | 6  | Midterm<br>CSTR equations for isothermal and non-isothermal  |
| 7  | Mixing and ideal reactor models (PFR, CSTR)—conversion and selectivity   | 7  | Multiple steady states in reaction systems   |
| 8  | Temperature effects in ideal reactors<br>Nonideal reactor models: mixing cell and dispersion   | 8  | Examples of real reaction systems:<br>Chlorination of Benzene<br>Oxidation of naphthalene<br>Ammonia synthesis   |
| 9  | Temperature effects in nonideal reactors<br>Reactions in two phases, mass transfer and reaction<br>Midterm III (mixing and ideal reactors)                               | 9  | Residence time distribution function, its utility and short-comings<br>Moving bed and fluidized reactors   |
| 10   | Introduction to some detailed simulation methods<br>Overview of course<br>Industrial example, catalytic cracking<br>Midterm IV (nonideal reactors) in lieu of final exam | 10   | External and internal diffusion in heterogeneous reaction systems,   |

... the student's analysis of kinetics is based purely on phenomenological rate laws with little understanding of their basis. Where does the Arrhenius law come from anyway? If we are careful to use activities in thermodynamic problems, shouldn't we use them in kinetics?

**TABLE 4.**  
Undergraduate Course, "Catalytic Reactor Design and Catalysis", University of California, Berkeley 3 hr/wk for 10 weeks.

| Week | Content  |
|------|--|
| 1    | Course Organization<br>Laboratory organization                     |
| 2    | Tutorials*<br>Preparation of Catalysts                             |
| 3    | Preparation of Catalysts<br>Physical Characterization of Catalysts |
| 4    | Reactor Design Principles  |
| 5    | Tutorials*<br>Reactor Design Problem                               |
| 6    | Reactor Design Problem<br>Rate Expressions for Catalysts           |
| 7    | Tutorials*<br>Rate Expressions, contd.                             |
| 8    | Homogeneous Catalysis<br>NO <sub>x</sub> reduction                 |
| 9    | Tutorials*<br>Fluidized Reactors                                   |
| 10   | Liquid-Liquid and Gas-Liquid Reactors<br>Student Reports           |

\*Tutorials by appointment, individually arranged.

#### EXPERIMENTS\*

- H<sub>2</sub>-D<sub>2</sub> Exchange**  
H<sub>2</sub>-D<sub>2</sub> exchange is measured on a fresh Ni film in a bulb using mass-spectrometer to analyze the progress of the reaction in a batch reactor.
- Hydrogenolysis of Cyclopropane**  
The kinetics of hydrogenolysis are studied in an integral packed bed reactor using Pt on  $\gamma$ -alumina catalyst. The objective is to determine experimentally reaction order and activation energy.
- Oxidation of Propylene**  
The objective is to determine activation energy for reaction of a dilute mixture of ethylene in air to CO<sub>2</sub> and water on a Pt-alumina catalyst. This experiment is an idealized model of an automobile catalytic converter.
- Esterification of Butyl Alcohol with Acetic Acid**  
The purpose of this experiment is to study the kinetics of esterification as affected by temperature, acidity, and effects of reversibility.
- Carbon-Carbon Dioxide Reaction**  
The reaction between graphite rods and CO<sub>2</sub> is studied at atmospheric pressure and at very high temperatures in a glow-bar furnace. The objective is to show directly the non-uniform reaction within the carbon rod.
- Oxidation on a Platinum Foil**  
The reaction of CO and O<sub>2</sub> is studied on an electrically heated platinum foil in a flow reactor. Reaction rates are determined from heat release on the catalyst. Reaction mechanism and activation energies are determined.

7. Catalyst Characterization  
BET surface area. Metal surface area.

8. Catalyst Preparation  
A typical catalyst is prepared by impregnating an alumina support with nickel salt. The nickel is reduced and subsequently the catalyst pellet is observed to establish the metal distribution.

\*Students do 2 experiments plus a catalyst characterization in addition to a reactor design.

experience need not be in terms of formal lecture courses, but may be in the form of research or journal reading seminars, special topics courses (whose content may vary from one year to the next), intensive mini-courses, etc. It is perhaps less appropriate here to become involved in a discussion of details of graduate courses at any level, since these ordinarily are much more reflective of the interests and experience of the instructor, and variations in content within wide limits are possible. Nonetheless, when we originally compared notes concerning the content of the entering level graduate courses at Berkeley and Northwestern we were struck by their similarity. These courses are basically a continuation in depth of the undergraduate courses, assuming background in descriptive kinetics and some understanding of ideal (PFR and CSTR) reactor models. One unifying theme in both courses is the discard of pseudo-homogeneous approximations and extensive treatment of reactions involving two phases. Under this cover we discuss heterogeneous catalysis, gas-liquid reactions, heterogeneous (two phase) reactor models, and the theory of diffusion and reaction. To our additional surprise, we found that considerable effort is devoted in both Northwestern and Berkeley courses to discussion of what might be termed "industrial examples". At Berkeley these include analysis of a FCC reactor-regenerator system and a study of the chlorination of benzene; at Northwestern kinetic lumping and decay models for catalytic cracking are investigated. Both courses also include a "sampler" on reactor stability and parametric sensitivity and introductory material on two-dimensional modeling. A syllabus of the Berkeley course is given in Table 5.

**TABLE 5.**  
**Graduate Course, "Chemical Reaction Analysis",**  
**University of California, Berkeley, 3 hr/wk**  
**for 10 weeks.**

| Lecture | Content  |
|---------|--|
| 1       | Orientation, organization, goals                                       |
| 2       | Stoichiometry, minimum independent variable in system                  |
| 3       | Conversion, definition of rate expression, conservation equations      |
| 4       | The problem of heterogeneous reactor design—the pseudohomogeneous rate |
| 5       | Langmuir-Hinshelwood kinetics  |
| 6       | Quasi-steady state methods   |
| 7       | Thiele-Zeldovich problem   |
| 8       | Falsification of kinetics by transport phenomena                       |
| 9       | Generalized treatment  |
| 10      | Heat effects, complex reactions, criteria                              |
| 11      | Parameters of model: BET area, metal area,                             |
| 12      | diffusivity  |
| 13      | Single pellet diffusion reactor  |
| 14      | Models of poisoning  |
| 15      | External mass transfer   |
| 16      | Reactor design, residence time distribution                            |
| 17      | Residence time distribution  |
| 18      | Application of RTD to reactor modeling                                 |
| 19      | Reactor-regenerator; fouling   |
| 20      | Examination  |
| 21      | Chlorination of benzene: example                                       |
| 22      | Stability: Van Heerden,  |
| 23      | Bilous and Amundson  |
| 24      | One-dimensional reactors   |
| 25      | Stability: $\text{NH}_3$ synthesis, Grens problem                      |
| 26      | Two-dimensional reactors   |
| 27      | Boundary conditions, hot spot example (phthalic anhydride)             |
| 28      | Fluidized reactors   |
| 29      | Slurry reactors  |
| 30      | Trickle-bed reactors   |

If this single example possesses any generality, it would tend to indicate that a degree of consensus exists concerning the lower level graduate course similar to undergraduate courses. Beyond this level, however, offerings become quite varied depending on the interests and resources of individual departments. Normally, one finds some course dealing with various aspects of detailed reactor design, such as two dimensional, two phase fixed beds, fluidized beds, slurry, or trickle bed reactors.

A final note concerning graduate education in

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this field is the high potential value of individualized seminar courses or research seminars. These can be organized about special topics and made complimentary to material presented in more formal courses. At Northwestern, for example, there is a rather sizeable group of individuals in ChE, Chemistry, and Materials Science who are involved in catalysis research. Faculty, students, and visitors participate in a "Catalysis and Surface Science" seminar approximately every other week amid the munching of potato chips at Friday noon. A typical schedule of speakers, affiliations, and topics is given in Table 6. This seminar series is a nice supplement to courses in advanced reaction kinetics and catalysis which are generally offered in the winter and spring quarters.

In summary, we see a large measure of agreement on the content of undergraduate and entering level graduate courses in chemical reactor engineering, as illustrated here. What of the future? Assuming that current research interests are

**TABLE 6.**  
**Catalysis and Surface Science Seminars**  
**Spring Quarter, 1977, Northwestern University**

1. Professor J. J. Fripiat, C.N.R.S., Orleans, France (visitor), "Aspects of Zeolite Catalysts: Evidence for Hydrogen Spillover"
2. Dr. R. Bjorklund, Dept. of Chemistry, Northwestern (post-doctoral fellow), "Properties of  $\text{Ni}/\text{Al}_2\text{O}_3$  Catalysts Prepared by Reaction of  $\text{Ni}(\text{CO})_4$  with Alumina"
3. Dr. M. Jarjoui, University of Lyons, France (post-doctoral fellow), "Partial Oxidation of Ethylene over Silver Catalysts"
4. Dr. Y. Inoue, Department of Chemistry, University of Tokyo (post-doctoral fellow), "The Reactivity of Supported Pt with  $\text{O}_2$ "
5. Professor J. B. Cohen, Department of Materials Science, Northwestern, "EXAFS and Its Applications in Surface Science"
6. Mr. D. M. Downing, Dept. of Chemical Engineering, Northwestern (graduate student), "Modeling Thermal and Mass Transport Interactions in Deactivated Catalyst Particles"
7. Mr. P. Otero-Schipper, Dept. of Chemical Engineering, Northwestern (graduate student), "Hydrogenation and Hydrogenolysis on Supported Pt"

going to show up in higher level graduate courses and thence diffuse downwards, we would expect to see increasing emphasis on unsteady state models, polyfunctional catalysis, catalyst deactivation, stability and sensitivity problems of various types, and lumping schemes for analysis of complex reaction networks. Can we be blamed if this sounds like a listing of our own research interests? □