A Course in

KINETICS AND CATALYSIS

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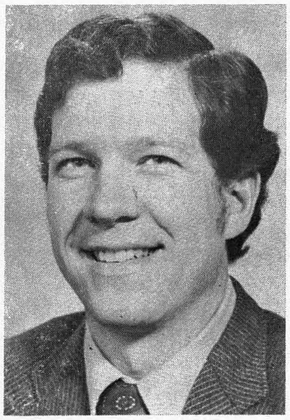
CATALYSIS IS A DEVELOPING SCIENCE which plays a critically important role in the petroleum, chemical, and emerging energy industries. It combines principles from somewhat diverse disciplines of kinetics, chemistry, material science, surface science and reaction engineering.

The subjects of kinetics and catalysis are very basic to graduate curriculums in Chemical Engineering and Chemistry. Yet because of the demanding nature of graduate curriculum requirements, few departments can afford the luxury of offering and/or requiring more than one introductory course treating a combination of these two subjects.

THE CHALLENGE

The challenge at BYU is to combine the fundamentals of kinetics and scientific/engineering principles of heterogeneous catalysis into a single-semester, 3-credit course suitable for chemical engineering and chemistry graduate students. A typical class consists of 15-20 students, most of which are M.S. and Ph.D. bound chemical engineers, the remainder consisting of 1-2 chemistry majors and 1-2 chemical engineering seniors. The obvious diversity in class makeup and subject matter requires (i) review of some basic kinetic and chemical principles and (ii) a careful compromise between depth and breadth in course topics. Accordingly the course is divided into eight topics covered in 35 50-minute lectures (see Table 1). In addition, three special lectures and three demonstrations (see Table 2) and a term paper based on study of the literature add spice and flavor to the course.

Another challenge which faces instructors of kinetics and catalysis is that of finding suitable text materials. There is, in fact, no single text which covers this subject matter as outlined in Table 1. Our solution to this dilemma is to use portions of J. M. Smith's book on "Chemical Engineering Kinetics" (the only required text) supplemented with 4 chapters from Boudart's "Kinetics of Chemical Processes" (out of print and used by permission from the author), reference books on library reserve and papers from the literature (see References).



Calvin H. Bartholomew received his B.S. degree in Chemical Engineering from Brigham Young University and his M.S. and Ph.D. degrees in Chemical Engineering from Stanford University. He spent a year at Corning Glass Works as a Senior Chemical Engineer in Surface Chemistry Research. In 1973 he joined the Chemical Engineering Department at Brigham Young University and is currently associate professor. His major research interests are heterogeneous catalysis (adsorption, kinetics and catalyst characterization), Moessbauer spectroscopy and air pollution chemistry.

COURSE ORGANIZATION

THE COURSE BEGINS WITH A brief but enthusiastic introduction to the world of catalysis and the basic concepts, rules and definitions of kinetics. The foundation for understanding and predicting reaction rates is next laid through 6

TABLE 1: Course Outline

I. INTRODUCTION AND DEFINITIONS (two lectures)
   A. Past, present and future of catalysis
   B. Basic kinetic concepts and definitions
II. KINETIC THEORY (six lectures)
   A. Collision theory
   B. Transition state theory
   C. The H_2 - I_2 reaction, a case study
   D. Thermodynamic formulation of rates
III. CONCEPTS, METHODS, AND TOOLS OF KINETICS (three lectures)
   A. Elementary steps/active centers and catalysis
   B. Catalysis and the steady state approximation
   C. Concept of the rate determining step
IV. ADSORPTION (four lectures)
   A. Adsorption processes and types
   B. Adsorption Isotherms
      1. Langmuir
      2. Others (Freundlich, Tempkin and BET)
   C. Chemisorption
      1. Measurement of Active metal surface area
      2. Calculations of dispersion and crystallite size
      3. Heterogeneity and particle size effects
V. KINETICS OF SURFACE REACTIONS
   A. Unimolecular and bimolecular surface reactions
   B. Kinetics of heterogeneous catalytic reactions
      1. Definitions of rate, activity, selectivity, and turnover number
      2. Facile and demanding reactions
VI. METHODS AND MATERIALS IN CATALYSIS (two lectures)
   A. Catalyst properties and materials
   B. Catalyst selection and testing
   C. Catalysts characterization—tools of the trade
VII. DIFFUSION AND MASS TRANSPORT IN CATALYSIS (seven lectures)
   A. Diffusion in porous catalytic solids
      1. Overall rates and resistances
      2. Effects of pore diffusion on rate—models and equations
      3. Pore resistance criteria
   B. Film mass transfer
      1. Model and correlations
      2. Calculation of k_m
      3. Mass transfer criteria
   C. Nonisothermal heat effects
VIII. REACTOR DESIGN IN HETEROGENEOUS CATALYSIS (eight lectures)
   A. Review of ideal reactors
   B. Material and energy balances for fixed beds
   C. Laboratory and industrial reactors
   D. Case study: reactor design of a methanator

lectures on kinetic theory using the magnificent work of John H. Sullivan on $H_2 + 2I \rightarrow HI$ as our classic case study. The student is next fitted with the basic tools of kinetics in three lectures dealing with elementary steps, the steady state approximation and the concept of rate determining step. Here the methanation of CO serves as our model reaction. The foundation and tools are now used to erect the course framework consisting of four lectures on adsorption and surface reactions, the most basic processes in catalysis. Two lectures on methods and materials in catalysis provide an interesting diversion while introducing the knowledge of catalyst structure needed to tackle the meaty subjects of diffusion and mass transfer. We concentrate on these latter subjects in some depth (seven lectures) and in a way which prepares the student for the ultimate engineering problem of designing fixed bed catalytic reactors. Again methanation is used as our model reaction.

LEARNING FROM EXPERIMENTS AND LITERATURE

A MOST ENJOYABLE PART of the course involves special lectures, experimental demonstrations (see Table 2) and the study of papers from the literature. The oscillating reaction is clearly our most dazzling demonstration; although the simple study of water level recession rates in a tank with the exiting tube either verticle or horizontal provides a rewarding kinetic analogy in connection with Bernoulli's equation. The very exothermic oxidation of ammonia on thin (brightly) hot Pt and Cu wires provides a fascinating but straightforward demonstration of the role of heat transfer in catalysis.

Because catalysis is in large part an experimental science, several class assignments are directed at understanding basic experimental techniques, methods of analyzing data, and elements of reactor design (including the design of a recycle methanator). Most of our weekly as-

TABLE 2

Special Lectures and Demonstrations

SPECIAL LECTURES

1. Kinetic Analogies
2. Oscillating reactions and auto catalysis
3. Catalytic petroleum refining processes

DEMONSTRATIONS

1. Kinetic analogy: Water level in a tank with outlet
2. Oscillating reactions
3. Hot wire ammonia oxidation

signments include the reading of a carefully selected journal article (see References). One of the assignments is to critically review one of these articles, a task which stimulates the thinking of the best students and makes for interesting class discussion. However, the assignment that appears to have the greatest learning impact is the preparation of a literature review paper on a topic of the students' choice, typically a catalytic reaction or process. □

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