

# CHEMICAL REACTION ENGINEERING SCIENCE

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**T**HE FOCUS OF the Chemical Reaction Engineering Science course at the University of Missouri-Columbia is on the theoretical description and interpretation of the phenomenological behavior of heterogenous catalysts. A student entering this course is presumed to have had at least a three hour course on chemical reaction engineering which covered the following topics:

- 1) Rate equations for homogenous reactions
- 2) Isothermal and temperature effects in the ideal batch, ideal plug flow, and the ideal stirred tank reactors
- 3) Characterization of non-ideal reactor performance by means of the residence time distribution, the dispersion model, the segregated flow model, and the tanks in series model
- 4) Heterogenous reactions and
- 5) Fluidized bed reactors. The course begins with a brief review of the batch, plug flow, and stirred tank reactors using a unified approach via the general material and energy balances expressed in terms of differential forms [1], i.e.—

$$L_v A = f \quad \text{Navier Stokes Equation}$$

$$i(v) L_v A = i(v) f \quad \text{Energy Equation}$$

$$dJ = 0 \quad \text{Conservation of Mass  
Equations}$$

The stability analysis and existence of bifurcation points for the nonlinear isothermal and adiabatic operation of the ideal reactors is made using the degree of a map and surface curvature concepts in the differential form language. The solutions for these nonlinear problems is developed using Green's function techniques. This approach has the advantage of introducing at the beginning of the course the general mathematical and physical framework needed to analyze phenomenological catalytic behavior.

At this point in the course the Langmuir-Hinshelwood [2] description of fluid-solid catalytic reactions is developed. The approach taken is to first consider the situation in which one step (mass transfer, adsorption, surface reaction, pore diffusion or, desorption) is controlling the overall reaction rate. The equations appropriate to each case are developed. Mass and heat transfer correlations are discussed where needed. When pore diffusion is taken up both the Thiele modulus and the effectiveness factor are defined. Various geometric shapes of the catalyst as well as temperature gradients within the porous catalyst are dealt with. Multiple controlling steps in the reaction process are then reviewed and the appropriate design equations obtained. The uniqueness and stability of the various descriptions of catalyst behavior are analyzed using the mathematical tools

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previously presented. Current papers in the catalytic literature where these methods are used is reviewed. It is pointed out at this juncture that the Langmuir-Hinshelwood approach does not in general lead to a unique physical interpretation of the experimental data but generally provides adequate design equations.

## FURTHER INSIGHT

**T**O FURTHER DEVELOP an insight into the physical process that occur during catalysis four final topics are considered in this course. They are: (1) geometric theory of catalysis, (2) the electron band theory of catalysis deals with

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In several places the progression from simple, quick and rough to detailed time-consuming and close estimates is dramatized. The laudable purpose here is to inspire students to develop judgement.

Also a note about the teaching of engineering economics is in order. In his preface, Woods notes: "many students undergo a long induction period before they appreciate some of the concepts". My experience confirms this view, but I would add that practicing engineers grasp the concepts readily, no doubt because they are familiar with business background and practice.

The initial chapter, *The Decision Makers*, is a vigorous view of the engineer in society, his responsibilities, and ethics in practice. Although the tone is idealistic, and perhaps naive, it is praiseworthy. A quote from the book is to the point "... engineers are, by and large, the decision makers in industry and technology . . ." (Actually we should be more influential than we are, but by nature we are less assertive than others, e.g., company managers).

The second chapter presents the economic environment. Basic economic concepts are covered: supply, demand, competition, cash flow, allocation of financial resources. Unfortunately, because of its brevity the treatment serves only to stress the need for such an overall perception.

The couching of the economic evaluation in terms of accounting practice is commendable. For cost data and for project authorization, we must deal with accounting and financial types, so engineers must speak the "accounting" language.

Outstanding merits of the work are the introduction of pertinent material from other fields, some novel approaches, homilies and examples designed to evoke engineering judgment, useful compendia of cost data, good specimen forms for the preparation of cost estimates, provocative problems, a valuable bibliography and an excellent glossary of relevant terms.

The book is compact, perhaps excessively so for the wealth of ideas, examples, tables, etc., which it contains. It has only 340 pages. For much of the material an extended, amplified treatment would be preferred, particularly in its service as a textbook. Its classroom use may require expansion on some topics in lecture by the instructor to derive the maximum benefit. This unique, diverse, rich, exciting book should also provide an excellent review or an introduction to this subject for practicing engineers. □

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the multiplet theory of Balandin [3] and the premise that the catalytic activity is determined by the compatibility of the catalyst surface geometry for the reaction being considered. The key ingredients are the lattice parameters and the arrangement of catalyst surface atoms which are correlated with catalytic activity. The electron band theory of catalysis [4] is principally applied to transition metal and alloys and seeks to relate catalysis, principally through the chemisorption step, to the electronic properties of the bulk solid. The subject of the electron theory of semiconductor catalysts represents a review of the work of F. F. Vol [1] and Kenshtein [5] on the role of the Fermi level in acceptor and donor reactions occurring on a semiconductor catalyst surface. The final topic, the charge transfer theory of catalysis, starts with a review of the work of Hanffe [6] and Lee [7, 8] on charge transfer reactions. The effects of D.C., symmetric A.C., and antisymmetric A.C. capacitively applied electromagnetic fields on the charge transfer catalytic reaction rate are discussed. The results of acoustically coupled phonon excitations on these same reaction rates are developed. Within this general context the effects of surface states (as distinct from the bulk energy states) on the catalytic processes that occur on transition metal oxides is considered [9, 10]. □

### REFERENCES

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