BOOKS

Proceedings of the Fifth International Congress on Catalysis, Joe W. Hightower (ed.), North-Holland Publishing Company, Amsterdam (1973). 2 volumes, 1,483 pages. $79.

These volumes contain the papers and discussions of the Fifth International Congress on Catalysis, held in Palm Beach, Florida, in August, 1972. The invited lecture by Ugo sounds a recurrent theme: coordination chemistry of organometallic complexes can illuminate chemisorption and surface reactions on transition metals and their oxides. Many of the papers point toward interpretations of catalysis by chemically identifiable surface species. This approach sets much of the current research apart from that of earlier congresses when researchers turned less often to surface chemistry and more often to solid state physics for explanations of heterogeneous catalysis.

Most of the research reported in the *Proceedings* is directed toward better understanding of particular catalysts, and it is convenient to arrange the papers by catalyst classes. Most catalysts were solids (for example, transition metal compounds and metals), but a few were used in the liquid phase, and some authors have developed ties between heterogeneous and homogeneous catalysis.

The most direct such tie is provided by organic and inorganic solids holding pendant transition metal complexes, as described by Allum et al. and Haag and Whitehurst. These solids offer the prospect of industrial application for processes like hydroformylation and carbonylation. They can be stable enough to eliminate problems associated with corrosion, separation of catalyst from products, and pollution of effluent streams. The accessibility of the attached complexes to study by spectroscopic means may allow reaction mechanisms to be discerned in the detail expected for reactions in solution (but not for reactions on heterogeneous surfaces) and provide the basis for molecular-scale catalyst design.

At the next level of complexity is the coordination chemistry of catalysis by surfaces containing transition metal ions in solid solution. The work of Cimino et al. and of Pepe and Stone illustrate the progress that can result from thorough characterization with catalytic reactions and spectroscopic methods. The latter authors found that Cr^{3+} ions incorporated at very low concentrations in an α-Al_2O_3 surface were efficient catalysts for dehydration of isopropanol by inducing the formation of strong Lewis acid sites in the immediately neighboring Al_2O_3 lattice. At higher concentrations, the Cr^{3+} ions interacted electronically, and the resulting delocalization of charge evidently facilitated the dehydrogenation of isopropanol.

Catalysis by transition metal oxides is especially well suited to investigation by electron spin resonance spectroscopy, and the work of Kazansky et al. illustrates application of the technique to CO oxidation catalyzed by V_2O_5 supported on silica. The data give evidence of the nature and surroundings of vanadium ions and identify the anion radicals formed from oxygen.

Solids with layer structures exemplified by MoS_2 and WS_2 have been often investigated as catalysts, yet only now that structures of many sulfides are well known is rapid progress being made toward understanding catalyst function. Farragher and Cossee have established the role of Co^{2+} and Ni^{2+} promoter ions intercalated between layers; intercalation of Ni^{2+} ions in the edges of WS_2 crystals leads to a reconstruction of the edges, giving a faceted surface with exposed W^{3+} ions, which are the catalytic sites for benzene hydrogenation. These results are important for understanding of industrial hydroprocessing catalysts like $CoO/MoO_3/\gamma$-Al_2O_3, which can be expected to find much increased application in hydrosulfurization of petroleum and coal.

Catalysis by zero-valent metals, especially Pt and Pd, continues to challenge the largest subgroup of researchers in heterogeneous catalysis. Among the most fruitful experiments have been those with alloys; Ponec and Sachtler used Cu/Ni alloys for reactions of hexane isomers, explaining their results in terms of electronic effects and catalysis by single surface metal atoms as well as ensembles of surface atoms. Many of the present papers concern catalysis by supported metals, demonstrating that some reactions (for example, certain hydrogenations) are structure-insensitive—proceeding at specific rates independent of the metal crystallite size—and others (for example, certain oxidations) are structure sensitive. Understanding of the crystallite size effects in terms of electronic and surface topographic properties (exemplified in the papers by Aben et al., Anderson and Shimoyama, and Oliver and Wells) is still not easily found. Notable for its absence is research with supported alloys, which have found application in improved industrial processes for catalytic reforming of petroleum.

Metals catalyze not just the familiar hydrogenation and hydrogenolysis reactions, but also partial oxidations. The most important industrial example is the oxidation of ethylene to give ethylene oxide catalyzed by supported silver. The paper by Kilty et al. demonstrates the advantage of using several well chosen experimental techniques in concert (infrared spectroscopy, isotopic tracer measurements, and chemisorption rate measurements) to elucidate the structures of surface species. A diatomic oxygen species chemisorbed on a single silver atom is necessary for selective oxidation of ethylene, whereas oxygen chemisorbed dissociatively on ensembles of four silver atoms is involved in oxidation of ethylene to CO_2.

Selective oxidation reactions are most often catalyzed in industrial processes by complex mixtures of metal oxides; one of the simplest examples is Bi_2O_3/MoO_3, which catalyzes the conversion of propylene to acrolein. The papers by Seiyama et al. and Moro-oka and Takita add details to mechanisms of partial oxidation reactions proceeding through allylic intermediates. The papers by Gorokhovatsky and Yurchak et al. concern little studied free-radical oxidations of liquid-phase reactants catalyzed by solids.

The solids most widely applied as catalysts and supports are aluminas. The contents of the *Proceedings* show a persistent interest in the complex surface chemical and catalytic properties of aluminas. Among the techniques, infrared spectroscopy and deuterium tracer studies have proven to be the most valuable, as demonstrated in the papers by Parkyns, Massoth and Kiviat, and Rosynek and Hightower.

Zeolites are high-area crystalline aluminosilicates used in large quantities for catalytic cracking; the molecular-scale pores of a zeolite are part of its crystal structure, and the uniqueness of zeolite pore sizes has allowed design of molecular shape-selective catalysts, a topic touched upon in the paper by Chen. The environments of the narrow zeolite pores have allowed preparation of stable clusters of perhaps as few as six metal atoms having catalytic properties distinct from those of metal crystallites found on amorphous solids, as discussed by Dalla Betta and Boudart. The role of hydrocarbon bridging compounds in facilitating the transport of hydrogen atoms from metal crystallites where they are formed to surfaces of zeolite supports is an important problem in bifunctional catalysis considered in the paper by Neikam and Vannice.

In a fraction of the papers, the emphasis is on new chemistry rather than catalytic function. New elements of hydrocarbon chemistry are described in the papers by Parravano (redistribution of carbon between cyclic paraffins) and Bhasin (intramolecular hydrogen transfer in olefins). Whan and Kemball and Hughes et al., respectively, have considered the little investigated topics of olefin disproportionation and molecular redistribution of paraffins and alkylbenzene.

Most of the papers we have cited concern catalysts and reactions bearing some relation to industrial processing, and there are many other good papers relating to ammonia synthesis, catalytic reforming, Ziegler-Natta polymerization, Phillips polymerization, and other processes. The great accomplishments in catalysis have been the process developments, and the *Proceedings* reaffirm the cliché that understanding follows the application in catalysis. The expected continuation of this pattern suggests future research emphasis on processes coming into prominence, and the present papers foretell the concern for reduction of nitrogen oxides, total combustion of hydrocarbons, and processing of fossil fuels to remove sulfur, nitrogen, and metals.

As chemical engineers, we are encouraged by the contributions of our colleagues to the *Proceedings* and to catalysis. We look ahead to increasing integration of chemistry into chemical engineering teaching and research and to more process synthesis which incorporates both design of reactors and plants and design of reactions at the molecular level.

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Computer Programs for Chemical Engineering, 7 Volumes, Aztec Publishing Company, P.O. Box, 5574, Austin, Texas.

These volumes were originally prepared by the CACHE Committee (Computer Aids for Chemical Engineering in Education) for use in chemical engineering education. They represent a tremendous collective effort by the editors and the contributors to put before chemical engineering educators tested programs that can serve in almost any type of course.

The specific volumes and their editors are

Volume	Editor	No. of pages	No. of computer programs	Cost
Stoichimetry	E. J. Henley	241	13	$11.95
Kinetics	M. Reilly	388	24	$13.95
Control	A. Westerberg	240	11	$11.95
Transport	R. Gordon	418	21	$13.95
Thermodynamics	R. Jelinek	350	15	$13.95
Design	R. Jelinek	400	11	$13.95
Stagewise Computations	J. Christensen	369	17	$13.95

Each of the volumes contains a number of problems that have been used by the respective contributors in their courses together with listings of the computer programs used to solve the problems. Most of the computer programs are fairly short so that they can be punched into cards without any difficulty. Problem statements and explanations range from two to twenty pages. Almost all the computer programs have ample documentation so that they can be used by the instructor and/or student without difficulty. A number of the programs not only have input and Fortran listings but also provide sample outputs so that the user can easily understand the results. Some of the problems include a brief statement of the pedagogical impact of the program including past usage, the concepts illustrated, and the objectives of the problem.

These volumes should prove extremely useful to anyone engaged in chemical engineering education. In addition, there are a surprising number of codes that could prove useful in industrial practice in the absence of suitable in-house computer library codes because, in addition to the codes in the design volume, there are many codes in the other volumes that can be helpful in process design.

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Computation for Process Engineers, G. L. Wells and P. M. Robson, Halsted Press, 192 pages. $12.75.

Computer systems are gaining widespread usage in the chemical process industries. But books describing their applications are slow to appear. Most books do not venture past the basic numerical methods and Fortran because interactions among input-output programs, data structures, and subprograms are difficult to describe in simple terms that do not over-emphasize computing in relation to process engineering. *Computation for Process Engineers* is one of the first books to dwell in this virgin territory. Its intent is to discuss the computational aspects of the problems presented in *Process Engineering with Economic Objective* by G. L. Wells.

The book's audience is difficult to define. It is either (1) the chemical engineering student and process engineer with limited background in Fortran programming, or (2) the process engineer with experience in the use and design of computing systems.

Computation for Process Engineers is a collection of chapters that review various aspects of computation. As an introductory text for students and process engineers, the coverage is often spotty and incomplete; many details are glossed over and computer jargon is commonplace. Experienced persons, on the other hand, would likely find the computation strategies too elementary and tersely presented. Most strategies are reviewed very briefly with references to the literature.

The book, in my opinion, might appeal to chemcial engineers who have limited knowledge of Fortran and seek exposure to the role of computing systems in process engineering. It would serve well as the basis for a two-day introductory course.

Chapter 1 defines computer terms: software, hardware, flow-charting, languages, and man-machine communication. But the definitions presume prior knowledge of the terms. I question whether this chapter might not best be omitted; excellent texts are available.

The categorization of unit computations in Chapter 2 is useful. The important point is that three kinds of programs are used to model process units: programs for material balances, material and energy balances and costing (short rating), and detailed design computations (full rating).

Chapter 3 reviews numerical and optimization methods. Methods for root-