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.

B. C. Gates
University of Delaware
Newark, Delaware 19711
and
E. Ruckenstein
State Univeristy of New York
Buffalo, New York 14214

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.

D. M. Himmelblau
University of Texas
Austin, Texas

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-

finding, solution of simultaneous linear equations, unconstrained optimization, and correlation of data are mentioned. Surprisingly, no mentions of simultaneous nonlinear equations or differential equations are made.

The objective of Chapter 4 is to "show the organization of unit computations." Unfortunately, the equations are not analyzed to prepare a solution procedure corresponding to a set of design variables, the Fenske-Underwood-Gilliland program does not appear in the Appendix as stated, and sophisticated simulation methods for distillation columns are reviewed only briefly.

Chapter 5 reviews the role of information flow diagrams in the analysis of process flow sheets and equation sets. In my opinion the methods for selecting design variables and tearing in the analysis of equation sets better belong in the preceding chapter.

Chapter 6 successfully demonstrates a step-wise procedure for the analysis of complex process flow sheets in the steady state. It reviews executive programs for material and energy balancing and costing. But a feeble attempt is made to describe the practical problems of data storage and transfer among physical property data, economic data, material balance programs, energy balance programs, sizing programs, and costing programs.

That the Fortran programs throughout the book are not well documented is surprising since the authors emphasize the importance of documentation to permit others to use programs. Poor documentation is particularly apparent in Chapter 7 on Generalized Optimization Problems, where a 50-step flow chart is summarized in one paragraph and is accompanied by three programs that are not clearly documented.

In summary, although *Computation for Process Engineers* is not a comprehensive book, it reviews any concepts that should be of interest to process engineers. The authors would do well to fill in the many holes and questions left unanswered in a subsequent text.

WARREN D. SEIDER
DEPT. OF CHEMICAL ENGINEERING AND COMPUTER SCIENCE
UNIVERSITY OF PENNSYLVANIA
PHILADELPHIA, PENNSYLVANIA

Vapor-Liquid Equilibrium Data Bibliography, I. Wichterle, J. Linek, E. Hala, American Elsevier, New York (1973). $47.50.

In 1968, the *Vapor-Liquid Equilibrium Data at Normal Pressures* by E. Hala, I. Wichterle and co-workers at

(*Continued in column 3*)

LETTERS TO THE EDITOR

TO THE EDITOR

In a recent paper by Hopper and Shigemura (1973), the kinetic rate constants and deactivation constants for the liquid phase isomerization of ortho-xylene over H-mordenite were reported. The deactivation constants were correlated by the exponential form:

$$B_i = B_{i0}\,\mathrm{EXP}(-\alpha_i\,[\theta/\tau]) \qquad (1)$$

where B_i is the rate constant for the ith reaction, B_{i0} the rate constant for fresh catalyst, α_i the deactivation constant, and θ/τ the feed-to-catalyst ratio. The authors evaluated the α_i and B_{0i} from the slopes and intercepts, respectively, of the ln B_i vs. θ/τ plots shown in Figure 11.

We draw your attention to the results reported in Table 4 for B_{i0} and α_i. The tabulated α_i are not consistent with the data shown on Figure 11 or the experimental B_i values tabulated in Table 3. In addition, the α_i should be positive if the exponential form in Equation (1) is assumed (that is, the catalyst deactivates with increasing θ/τ).

We have calculated the α_i and B_{i0} from the B_i data listed in Table 2 using linear least squares. Our calculated results appear in Table 1. Our results are also consistent with results calculated from the slopes and intercepts of the linear plots in Figure 11.

TABLE 1. DECAY MODEL CONSTANTS FOR ORTHO-XYLENE ISOMERIZATION

	α_i	$B_{i0} \times 10^6$ (m³/kg—s)	Residual
B_1	0.0195	0.156	8.06×10^{-16}
B_2	0.0196	0.178	1.03×10^{-15}
B_3	0.0522	2.982	1.93×10^{-14}
B_4	0.0523	1.153	2.88×10^{-15}
B_5	0.0615	1.224	3.38×10^{-15}
B_6	0.0612	2.771	1.78×10^{-14}

LITERATURE CITED

Hopper, J. R., and D. S. Shigemura, "Kinetics of Liquid Phase Xylene Isomerization over H-Mordenite," *AIChE J.*, 19, 1025 (1973).

ALAN M. KUGELMAN AND FRANCIS M. DEANE
DEPT. OF CHEMICAL ENGINEERING
UNIVERSITY OF MARYLAND
COLLEGE PARK, MARYLAND 20742

REPLY

The α_i values reported in Table 4 of our paper are incorrect as observed by Kugelman and Deane. The α_i values should be positive with numerical values of $\alpha_i = \alpha_2 = 0.0253$; $\alpha_3 = \alpha_4 = 0.0522$; and $\alpha_5 = \alpha_6 = 0.0614$ as originally reported by us in New Orleans (74th National AIChE meeting March 11-15, 1973). The values of Kugelman and Deane confirm our original values except for $\alpha_1 = \alpha_2$ and B_{01} and B_{02}. The disagreement is due to a difference in data interpretation. The values of α_1 and α_2 given above and the B_{01} and B_{02} in Table 4 are based on neglecting the value of B_1 and B_2 at $\theta/\tau = 15$ which is our best interpretation of the information because these latter values are not consistent with the trend of all the other information. Inclusion of this point will result in their values.

J. R. HOPPER AND
DENNIS S. SHIGEMURA
DEPT. OF CHEMICAL ENGINEERING
LAMAR UNIVERSITY
BEAUMONT, TEXAS 77710

BOOKS (*Continued*)

the Institute of Chemical Process Fundamentals in Prague was published. The same group has now published another valuable reference source book to document literature sources for vapor-liquid equilibrium data. A literature search from 1900 through 1972 showed that some 4800 papers reported V-L-E data. These citations were processed on a computer and tables prepared to allow a user to search for pertinent references applicable to any defined mixture. The Hill system used in the Chemical Abstracts formula index was employed to prepare the lists.

Trial searches made by this reviewer were carried out quickly and efficiently. No comments are provided as to the reliability of any reference; the value of this source is simply to locate the original reference. As such, it should be of real utility, especially to process design engineers who need data on particular systems. Even a null result is of value, at least one will know he did not overlook a reference!

ROBERT C. REID
MASS. INSTITUTE OF TECHNOLOGY
CAMBRIDGE, MASS. 02139