

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.

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**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:

$$B_i = B_{i0} \text{EXP}(-\alpha_i [\theta/\tau]) \quad (1)$$

where  $B_i$  is the rate constant for the  $i$ th reaction,  $B_{i0}$  the rate constant for fresh catalyst,  $\alpha_i$  the deactivation constant, and  $\theta/\tau$  the feed-to-catalyst ratio. The authors evaluated the  $\alpha_i$  and  $B_{i0}$  from the slopes and intercepts, respectively, of the  $\ln B_i$  vs.  $\theta/\tau$  plots shown in Figure 11.

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

We have calculated the  $\alpha_i$  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

	$\alpha_i$	$B_{i0} \times 10^8$ ( $\text{m}^3/\text{kg-s}$ )	Residual
$B_1$	0.0195	0.156	$8.06 \times 10^{-16}$
$B_2$	0.0196	0.178	$1.03 \times 10^{-15}$
$B_3$	0.0522	2.982	$1.93 \times 10^{-14}$
$B_4$	0.0523	1.153	$2.88 \times 10^{-15}$
$B_5$	0.0615	1.224	$3.38 \times 10^{-15}$
$B_6$	0.0612	2.771	$1.78 \times 10^{-14}$

### LITERATURE CITED

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

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### REPLY

The  $\alpha_i$  values reported in Table 4 of our paper are incorrect as observed by Kugelman and Deane. The  $\alpha_i$  values should be positive with numerical values of  $\alpha_1 = \alpha_2 = 0.0253$ ;  $\alpha_3 = \alpha_4 = 0.0522$ ; 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  $\alpha_1$  and  $\alpha_2$  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.

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### 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!

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