

Chemistry of Catalytic Processes, by Bruce C. Gates, James R. Katzer, and G. C. A. Schuit. McGraw-Hill, 1979, 464 pp. \$28.50.

This book treats the subject of catalysis from the viewpoint of both chemical engineers and chemists. The authors consider a number of industrially important catalytic processes from the standpoint of the basic chemistry involved as well as the engineering features which are important in commercial practice. The processes discussed include catalytic cracking, catalytic reforming, and hydrodesulfurization of petroleum fractions. Also included are partial oxidation processes and a variety of processes employing transition metal complexes as catalysts. The treatment includes discussions of reaction mechanisms, kinetics, and re-

actor design. Material is presented which will be of interest to workers whose activities range from process development to exploratory or basic research in catalysis. The book is written at a level which is well within the grasp of advanced undergraduates or beginning graduate students in chemical engineering or chemistry. It should be of interest primarily as a reference book rather than as a basic textbook, although it could be used effectively in a specialized course such as the short course which has frequently been conducted by the authors. For this latter purpose the authors have included a number of useful problems at the ends of the various chapters.

It is difficult to treat the subject of catalysis in a single volume, with a good balance between overall perspective and an adequate amount of detail.

The authors have succeeded in balancing their treatment in the individual chapters, each of which is concerned with a particular process or class of processes. However, it would have been helpful if the authors had included an introductory chapter considering catalytic processes in a general way, i.e., considering features common to all catalytic reactions and processes. While such an introductory chapter would have unified the presentation, its omission does not detract seriously from the book. Overall, the book is a useful addition to the literature of catalysis.

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LETTERS TO THE EDITOR

To the Editor:

Grevillot and Tondeur are to be congratulated on their very readable article 'Equilibrium Staged Parametric Pumping' [*AIChE J.*, 22, 1055 (1976)]. It is important that new or novel separation techniques reach as wide an audience as possible. One method of accomplishing this is to show simplified analogies with classical unit-operations such as these authors have done with a McCabe-Thiele representation of batch parametric pumping.

By using a stage-concept to represent a packed column configuration, the authors uncover some interesting results relating to the *limit regime* (ultimate steady state). The authors suggest the limiting separation depends for example, on the shape of the non-linear isotherms, on the spacing between them (temperature difference) and most especially on the number of stages assumed to represent the bed. At first glance, it may appear that prediction of limiting separation is at odds with the theory of ultimate separation we published at an earlier date (Foo and Rice, 1975; Rice, 1976),

with subsequent modifications (Foo and Rice, 1977). However, it is well known (see for example Gupta and Sweed, 1973) that the number of effective stages needed to represent a packed bed configuration depends on the magnitude and type of dispersive forces acting. Thus if axial mixing is violent or mass transfer coefficient is small, only a few stages might represent a finite, but long packed bed. In our work (which, we are sad to report, was not mentioned by Grevillot and Tondeur), the dissipation effects arising from intraparticle diffusion (the strongest effect), film resistance and axial mixing are combined in a unified theory to predict ultimate steady-state (or limiting regime). In most cases, an asymptotic form of the general theory (Rice, 1976) can be used for design purposes when proper account is taken of the initial charge composition (i.e. the constant mass condition, Foo and Rice, [*AIChE J.*, 23, 120 (1977)]). The continuum theory (as opposed to a stage-concept) includes the proper length and time scales needed for design purposes.

While a stage theory is appealing for its simplicity, it cannot be used for a priori predictions or design of packed parapumps until there is uncovered a fundamental relationship to compute HETS in such periodic adsorptive-desorptive systems.

To illustrate the approximate equivalence of the two results it is easy to show that the McCabe-Thiele Representation for N stages under conditions of linear equilibria is (c.f. Grevillot and Tondeur, Eq. (11)):

$$x_1 = (\alpha/\alpha')^N x_{N+1} \quad (1)$$

or defining the ultimate separation factor as

$$\alpha_\infty = x_1/x_{N+1} \quad (2)$$

there results

$$\ln(\alpha_\infty) = N(\ln \alpha/\alpha') \quad (3)$$

We may estimate a value of N corresponding to a packed bed with axial dispersion (after Klinkenberg and Sjenitzer (1956), which was originally suggested by Kramers and Alberda (1953) for simple tube flow) to give:

$$N \simeq Lv/2D_T \quad (4)$$

where here molecular diffusion is replaced with an effective total dissipative effect. Inserting this into Eq. (3), we see that separation factor depends exponentially on length, exactly as predicted by Foo and Rice, 1975.

Furthermore, it has been shown (Gupta and Sweed, 1973) combined dissipation effects under conditions of linear isotherms can be represented by

$$D_T = D + \frac{v^2 \bar{\alpha}^2}{h(1 + \bar{\alpha})^2} \quad (5)$$

where h is a mass transfer coefficient, D is axial dispersion coefficient and $\bar{\alpha}$ is an average slope of the linear adsorption isotherm. Taking axial dispersion as being linearly related to velocity (Klinkenberg and Sjenitzer, 1956) and assuming a constant transfer coefficient (slow flow) a combination of Eq. (3), (4), and (5) gives a simple linear connection with fluid velocity:

$$1/\ln \alpha_s = av + b$$

the form of which was predicted by Foo and Rice using an entirely different approach.

Clearly, the representation uncovered by Grevillot and Tondeur is a breakthrough, not only because non-linear isotherms can now be easily handled, but because their method is easy to understand and to apply. More work will be needed, however, to uncover a Murphree-type stage efficiency which reflects the unique dispersive force associated with solid or pore diffusion phenomena which so often limit adsorptive based systems (Rice, 1976, p163). In the final analysis, it is column length for a given separation which must be predicted.

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Reply:

We should like to insist on a few points, some of which we thought were clear in the scope and conclusion of our paper.

1. Parametric pumping is not restricted to packed beds, and can actually be performed in physically staged

cascades, such as, stirred tanks containing an adsorbant, in the way described in our paper.

2. Our staged model was *not* presented for the purpose of representing packed beds, but physically staged configurations. In such, it is the number of stages that is sought, in the final analysis.

3. One reason for this limitation is the restriction to a *single* transfer per half-cycle, which amounts to imposing a value of the "penetration" or "relative displacement," whereas this parameter is free in usual packed bed parapumps.

4. *Only within* this restriction is the ultimate separation factor given by Fenske's equation:

$$\alpha_s = (\alpha/\alpha')^N$$

with $\alpha_s = x_1/x_{N+1}$ if the isotherms are linear (equation 3 in Rice's letter)

$$\alpha_s = \frac{x_1}{1 - x_1} \bigg/ \frac{x_{N+1}}{1 - x_{N+1}}$$

if the isotherms are mass action type (equation 11b in our paper).

5. In *AIChE J.*, 23, 840 (1977), we extend the staged approach to multiple transfers per half-cycle (thus varying the penetration), a situation more likely to be related to packed bed analysis. If the concentration distribution exiting at each end of the column are conserved before being reinjected, by using a cascade of reservoirs, the separation factor shows an exponential dependence on number of stages N and on number of transfers n :

$$\alpha_s = \left(\frac{\alpha}{\alpha'} \right)^N \left(\frac{\alpha}{\alpha'} \frac{\rho + \alpha'}{\rho + \alpha} \right)^{n-1}$$

(for linear isotherms)

In the analogous packed bed situation, one might then expect an exponential increase with bed length and penetration. In the case of mixing and averaging of the exiting solution at each half-cycle (the situation studied by almost all previous workers, including Foo and Rice), no simple relationship is predicted by our model, but separation decreases about exponentially when penetration increases, which agrees with equation 6 of Foo and Rice, originally derived with penetration as a variable, instead of fluid velocity.

6. We do try to obtain usable results on packed bed parapumps from the staged approach, but some unsolved problems stand in the way. In particular the correspondence between staged models and axial dispersion models for such cyclic processes is not as clear cut as for simple tube flow.

To conclude, in the present state of the art, the staged model can be used as a *conceptual and qualitative* model for both packed bed and staged parapumps, but as a *design* model for the latter only.

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ERRATA

In "Simulation of the Dynamic Behavior of Deep Bed Filters" by Chi Tien, Raffi M. Turian and Hemant Pendse [*AIChE J.*, 25, 385 (1979)] the footnote should read "Raffi Turian is presently at the Department of Chemical Engineering, Texas Tech University, Lubbock, Texas 79409".

In "A Sparse Computation System for Process Design and Simulation: Part II. A Performance Evaluation Based on the Simulation of a Natural Gas Liquefaction Process" by R. S. H. Mah and T. D. Lin [*AIChE J.*, 24, 839 (1978)] the sentence beginning l. 39, left column, p. 847 should read: The iterations were terminated if either the Euclidean norm of the weighted residuals,

$$\left\{ \sum_{i=1}^n [w_i f_i(x)]^2 \right\}^{1/2}$$

was less than 10^{-6} or the numerical value of the ratio of the change of a variable to its present value was less than 10^{-8} for every variable. The weights are given in Table 4. Convergence was attained after six, eight, six and nine iterations for the four cases, respectively.

TABLE 4. WEIGHTS IN THE RESIDUAL NORM EVALUATION

Equation number	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
w_i	1	α_{ik}	1	$1/F$	$[G\pi(1 - \lambda_k)]^{-1}$ k	$[G\pi\lambda_k]^{-1}$ k	$1/G$	$[G\pi(1 - \lambda_k)]^{-1}$ k	$[\pi(1 - \lambda_k)]^{-1}$ k	1