

LETTERS TO THE EDITOR

To the Editor:

Recently Chang (1982) reported a numerical method for the estimation of the effectiveness factor for catalyst particles of high Thiele modulus with the Michaelis-Menten type kinetics. The report by Lakshmanan (1983) suggested a collocation method with a trial function for the concentration gradient near the catalyst surface. Both methods require a trial and error procedure. In this letter, a simple method using the general modulus (Bischoff, 1965) is suggested and shown to be useful in obtaining the effectiveness for catalyst particles of high Thiele modulus.

According to Bischoff (1965), the general modulus, M , with Michaelis-Menten kinetics, is

$$M = L \left(\frac{V_{\max}}{2DK_s} \right)^{1/2} \left(\frac{S_i}{K_s + S_i} \right) \times \left(\frac{S_i}{K_s} - \ln \left(1 + \frac{S_i}{K_s} \right) \right)^{-1/2} \quad (1)$$

where S_i is the concentration of substrate on the catalyst surface and L is the distance measured from the surface (at L , $dS/dr = 0$). In the case of high Thiele moduli, the curvature effect on the mass transfer rate in a spherical catalyst particle can be assumed negligible. This is a valid assumption when the thickness of "effective reaction zone" (Paterson and Cresswell, 1971) is very small relative to the particle radius, R , due to a high Thiele modulus. When the above conditions are met, the overall reaction rate per catalyst particle, $\hat{\gamma}_{\text{overall}}$, can be written (Bischoff, 1965; Moo-Young and Kobayashi, 1972) as

$$\hat{\gamma}_{\text{overall}} = \left(\frac{1}{M} \right) (4\pi R^2 L) \left(\frac{V_{\max} S_i}{K_s + S_i} \right) \quad (2)$$

$$= 4\pi R^2 \sqrt{2DK_s V_{\max}} \times \left(\frac{S_i}{K_s} - \ln \left(1 + \frac{S_i}{K_s} \right) \right)^{1/2} \quad (3)$$

We can express the concentration of substrate on the catalyst surface (unmeasurable) as

$$S_i = S_o - \frac{\eta}{\frac{3k}{R} \left(\frac{K_s + S_o}{S_o V_{\max}} \right)} \quad (4)$$

Inserting Equation (4) into (3) and using the dimensionless variables defined previously (Chang, 1982; Lakshmanan, 1983), we can derive the implicit function with respect to η as follows

$$\eta = \frac{3\sqrt{2}}{\phi} (1 + \beta) \left[1 - \frac{\eta \phi^2}{3Sh(1 + \beta)} - \beta \ln \left(1 + \frac{1}{\beta} \left(1 - \frac{\eta \phi^2}{3Sh(1 + \beta)} \right) \right) \right]^{1/2} \quad (5)$$

Equation (5) is the working equation for the

TABLE 1. VALUES OF η FOR $\phi = 100$

| η values | $Sh = 100; \phi = 100$ | | |
|--|------------------------|---------------|---------------|
| | $\beta = 0.01$ | $\beta = 0.1$ | $\beta = 1.0$ |
| (a) Chang (1982) | 0.0215370 | 0.0211400 | 0.0277893 |
| (b) Nine point collocation (Lakshmanan (1983)) | 0.0215358 | 0.0211169 | 0.0275801 |
| (c) This work | 0.021584 | 0.021180 | 0.027779 |
| % difference $\left(\frac{(b) - (a)}{(a)} \times 100, \text{ nine point collocation} \right)$ | -0.01% | -0.11% | -0.75% |
| % difference $\left(\frac{(c) - (a)}{(a)} \times 100, \text{ this work} \right)$ | 0.22% | 0.19% | -0.04% |

determination of η with given β , ϕ and Sh .

The values of η calculated with Equation (5) compare very well with the values reported for the case of $\phi = 100$. (Chang, 1982; Lakshmanan, 1983). These are shown in Table 1.

As can be seen the η values calculated from Equation (5) agree very well with the values of numerical calculations (Chang, 1983) and with those by nine point collocation (Lakshmanan, 1983). The calculation of η with Equation (5) is straightforward and does not require trial and error. In conclusion, Equation (5) can be used successfully in calculating the effectiveness factor for catalyst particles of high Thiele modulus with the Michaelis-Menten type kinetics (or the Langmuir type, or the Monod type).

NOTATION

| | |
|----------------|--|
| D | = diffusion coefficient |
| k | = external mass transfer coefficient |
| K_s | = Michaelis-Menten constant |
| L | = distance measured from the surface to the inside of the particle |
| M | = general modulus |
| r | = radial coordinate |
| $\hat{\gamma}$ | = reaction rate |
| R | = radius of a catalyst particle |
| S_i | = the concentration of substrate on the catalyst surface |
| S_o | = the concentration of substrate in bulk stream |
| Sh | = Sherwood number |
| V_{\max} | = maximum reaction rate |

Greek Letters

| | |
|---------|------------------------|
| β | = saturation constant |
| η | = effectiveness factor |
| ϕ | = Thiele modulus |

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- Lakshmanan, C., "To the Editor," *AIChE J.*, **29**, 876 (1983).
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JUAN HONG
Department of Chemical and Nuclear Engineering
University of Maryland
College Park, Maryland 20742.

Reply:

We thank Lakshmanan (1983) and Hong for their interests in the article concerning a numerical scheme at high Thiele moduli. Both their comments are correct in their own sense and helpful for showing various aspects of the problem. But the article was prepared under the idea of proposing a numerical scheme suitable for stiff problems with the inner region of a boundary layer type (Nayfeh, 1973). Since solution of the outer region is generally given in an analytical form, it can be used as a starting point for seeing the profile of the inner solution, or the solution of the whole domain in the end.

If calculation of the effectiveness factor for the Michaelis-Menten Kinetics at high Thiele moduli was only an object of the article, we would rather have suggested the following relation (Ghim and Chang, 1983):

$$\eta = \frac{s\sqrt{\beta}}{\phi} (B + 1) \left[\left(\frac{\phi}{Sh\sqrt{\beta}} + 1 \right) \beta + \frac{1}{3} \left(\frac{Sh\sqrt{\beta}}{\phi + Sh\sqrt{\beta}} \right) \right]^{-1} \quad (1)$$

The values of η calculated by Eq. 1 at $s = 3$, $\phi = 100$ and $Sh = 100$ are 0.0215961, 0.0210261, 0.0276923 for $\beta = 0.01, 0.1, 1.0$, whose errors relative to those by Chang (1982) are 0.27%, -0.54%, -0.35%, respectively. These are somewhat loose compared with those by Hong, but much better than the results from one point collocation by Lakshmanan (1983). The strong point of Eq. 1 is apparent that the relation is simple, fully explicit and sufficiently accurate at high Thiele moduli.

Notation

s = shape factor, 3 for a sphere, 2 for a cylinder and 1 for a slab geometry
 Sh = Sherwood number
 β = Michaelis-Menten constant
 η = effectiveness factor
 ϕ = Thiele modulus

Literature Cited

- Chang, Ho Nam, "Numerical Calculation of Effectiveness Factors High Thiele Moduli" *AIChE J.*, **28**, 1030 (1982).
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HO NAM CHANG

Department of Chemical Engineering
 Korea Advanced Institute of Science and Technology
 Cheongryang
 Seoul, Korea.

To the editor:

In a recent *R & D Note* Kawase and Ulbrecht [*AIChE J.*, **29**, 689, (1983)] attempted to develop an asymptotic boundary layer solution for high Schmidt number mass transfer, however they used an incomplete form of the thin concentration boundary layer equation. Under the approximations of constant properties and $Sc \rightarrow \infty$ the species continuity equation becomes

$$u \frac{\partial y}{\partial x} + v \frac{\partial c}{\partial y} = D \frac{\partial^2 c}{\partial y^2} \quad (A)$$

where v is the velocity normal to the surface. The other symbols are defined by Kawase and Ulbrecht. In their Eq. 1 the term involving v has been dropped although it is of the same order of magnitude as the term involving u . When a profile for u is assumed, the overall continuity equation is used to obtain v .

The analysis leading to Eq. (A) and the analytical solution of this equation were first published by Lighthill (1950). Similar analyses were published for spheres (Baird and Hamielec, 1962) and for axisymmetric bodies (Lochiel and Calderbank, 1964).

Acrivos *et al.* (see the original *Note* for references not listed here) were the first to introduce the Lighthill method to the chemical engineering literature. At the same time Carberry and co-workers, apparently unaware of the Lighthill and Acrivos results, applied Eq. 1 of the *Note*. Since closed form solutions can be obtained to the correct asymptotic equation, there is no need to use Eq. 1 and the approximate analysis of the *Note*.

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Martin E. Weber

Department of Chemical Engineering
 McGill University
 Montreal, Quebec, Canada.

Reply:

Dr. Weber is, of course, right that the complete form of the thin boundary layer equation is more rigorous than the one used in our note. He has not, however, realized that a more rigorous equation need not always lead to a more rigorous solution. For the flow past a sphere, Equation (A) of his letter applies only to the separation point but not beyond it. The mass transfer in the wake must be approximated by implying different mechanisms of transport and some of the authors cited in Dr. Weber's letter (Lochiel and Calderbank) simply estimated the transfer rate in the wake. In light of this, the error caused by the omission of the normal convective term in Eq. (A) is likely to be far less than that due to the wake approximations.

Further, even for the mass transfer from

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a flat plate, where there is no boundary layer separation the omission of the normal convective term in Eq. (A) leads to only 18% to 20% overestimation of the Sherwood number in the range of flow indices between 1.6 to 0.3.

Having this in mind, it comes as no surprise that the model of Mixon and Carberry (cited in our note) does such a good job for the mass transfer in a bed of fixed spheres where the flow pattern is made very complex by the existence of wakes and interparticle interactions.

Finally, we would like to use this opportunity to point to a misprint in the $A_1(n)$ term of our note. The exponent in the square bracket should be $(2-n)(n+1)$ rather than $(2-n)(m+1)$.

J. J. Ulbrecht and Y. Y. Kawase
State University of New York at Buffalo
Buffalo, N.Y. 14260.

To the editor:

On "Degree of Segregation and Coalescence Rate Parameter in the Random Coalescence Model for a Stirred Reactor" [*AIChE J.*, 29, 513 (1983)]

We appreciate Professor Curl's interest [*AIChE J.*, 29, 878 (1983)] in our note, where Dankwerts' degree of segregation, J , for the random coalescence model of mixing has been calculated by Monte Carlo simulation as a function of the coalescence rate parameter.

We must remark, however, that the analytical derivations quoted by Professor Curl in his letter (Verhoff, 1969; Komasaawa *et al.*, 1971; Ross *et al.*, 1978) all refer to variance of concentration rather than to variance of age. Hence the result of these authors should be identified as the intensity of segregation (component segregation), I_s , based on component fraction, and not as the degree of segregation, J , based on age. The same analytical result was obtained by Evangelista *et al.* (1969) and discussed in our note.

Dankwerts (1958), Brodkey (1966, 1967) Rao and Edwards (1973), Takao and Murakami (1976), Takao *et al.* (1979), Nauman (1981) are among the authors who clearly distinguished between component segregation and degree of segregation based on age, although "the use of the same general terminology for the very different physical process of mixing and self-mixing (or back-mixing) has led to some confusion" (Brodkey).

Takao and Murakami (1976) derived analytical expressions for I_s and J for several models of micromixing and concluded that they may or may not coincide depending on the model.

P. F. Marcom and N. Vatistas
Department of Chemical Engineering
University of Pisa
Pisa, Italy 56100

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ERRATUM

In "Bubble Formation at Vibrated Orifices: Medium-Chamber-Volume Region" [*AIChE J.*, 30, 37 (1984)] the author's names should read C. T. Barker and Noel de Nevers.

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