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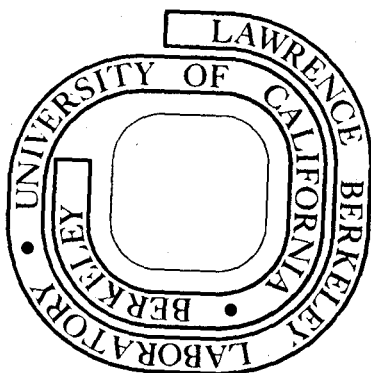
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Low Péclet Number Behavior of the Transfer Rate
in Packed Beds

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Abstract

The asymptotic behavior of the mass-transfer coefficient in a packed bed reactor at low Péclet numbers is dependent upon how the coefficient is defined. A singular perturbation approach coupled with heuristic arguments is used to demonstrate that the film mass-transfer coefficient in deep beds approaches a constant value as the Péclet number decreases. The film coefficient is utilized in the one-dimensional model of a bed as a sink term in the governing equation. The volumetric, or effective, mass-transfer coefficient which relates the overall reactant conversion to a logarithmic mean concentration driving force, decreases linearly with the Péclet number as the Péclet number approaches zero. The distinction between the two coefficients is important in the low Péclet number region. Analogous results apply to heat transfer. Reported experimental data support these predicted trends.

Introduction

The behavior of the particle-to-fluid (or vice-versa) heat or mass transfer rate in packed beds at low Péclet numbers has been a source of confusion in the chemical engineering literature. The question is, "Does the transfer rate approach a steady value as the Péclet number decreases, or does it continually decrease with the Péclet number?" This can be rephrased by asking whether the Sherwood number reaches a constant value or decreases as the Péclet number is lowered. We shall demonstrate in this paper that both trends are possible depending upon how the Sherwood number is defined.

The experimental determination of transfer coefficients at low Péclet numbers is vexing. The fluid leaving the bed is very near its saturation value in the transferred quantity. This creates a large uncertainty in the driving force at the exit of the bed which is used in defining the effective transfer coefficient. Free convection may also become an important effect. To overcome these difficulties, various workers have used diluted beds, transient, and frequency response methods to determine more accurately the low-Péclet-number behavior.

Since the Schmidt and Prandtl numbers for liquids are quite large [$0(10^3)$], most low Péclet number data are found in gaseous systems. Furthermore, most workers have varied the Reynolds number only. The free convection effects should be minimized in the gaseous systems.

The quantity of data for low Péclet numbers is understandably small. Table I is a compilation (with no claim to completeness) of

those publications which list packed-bed transfer data for Péclet numbers less than 30. Both heat and mass transfer results are included. The data scatter as the Péclet number decreases, and there is no absolute agreement between different authors. (This is true, to an extent, no matter what the Péclet number range.) There is, however, a definite trend in the Sherwood number (or equivalently, the Colburn j factor) with the Péclet number reported by the authors of Table I. The Sherwood number based on an averaged inlet and outlet concentration (or temperature) driving force across the bed (3,6,7,9,13,25,28,31) seems to decrease with the Péclet number. However, the film Sherwood number (10,17,21,22,23) seems to reach a constant as the Péclet number decreases. The film Sherwood number is calculated by parameter fitting the experimental data to the solution of the governing one-dimensional convective diffusion equation.

A concise definition of these two different Sherwood numbers follows. We shall demonstrate that the distinction between these two numbers is small for large Péclet numbers but becomes important as the Péclet number approaches zero.

Definitions of the Mass-Transfer Coefficient

To be specific in our discussion, we shall speak in terms of the mass-transfer problem in a nonconsolidated packed bed. The results are applicable to the heat-transfer problem by the usual analogies. We shall also limit our discussion to a single reaction at the particle surfaces. The rate of reaction is controlled by the reactant mass transfer from the fluid to the particle surface.

A design engineer is interested in the performance capabilities of a packed bed reactor. Given a certain feed concentration of reactant, he is interested in the overall reactant conversion. This can be correlated in terms of the bed's effective mass-transfer coefficient k_m .

$$v[c_F - c_L] = ak_m L \Delta c_{\ln} \quad (1)$$

The concentrations c_F and c_L are the far upstream and downstream reactant concentrations. Equation 1 relates the conversion to a logarithmic mean driving force. (Some workers have chosen different driving forces. Bird et al. (4) give a lucid discussion of the possibilities.) For the limiting reactant condition considered here, equation 1 reduces to

$$\frac{c_L}{c_F} = \exp \left(- \frac{Sh_B}{Pe_B} \frac{aL}{\epsilon} \right) \quad (2)$$

where the bed Sherwood and Péclet numbers have been introduced.

It is also possible to define a film coefficient k_f . This coefficient relates the local concentration driving force in the bed to the local reaction rate. It is assumed for a given flowrate that k_f does not vary throughout the bed. The term $(k_f c)$ appears as a sink term in the one-dimensional equation governing the concentration profile in the bed:

$$E \frac{d^2 c}{dz^2} - v \frac{dc}{dz} = ak_f c. \quad (3)$$

The dispersion coefficient E is a function of the flow regime. In the limit of low Péclet numbers, E is dominated by molecular diffusion and reduces to

$$E = \epsilon \frac{D_o}{\tau}$$

where ϵ is a tortuosity factor (32).

It might seem that k_f is a more fundamental quantity than k_m (or vice-versa, depending upon one's point of view). This is not so, however, since both k_m and k_f are essentially defined quantities. These two coefficients are related. This can be seen by solving equation 3 with appropriate boundary conditions to find the concentration field across the bed. After solving this expression for c_L/c_F and setting this result equal to equation 2, one obtains (26)

$$k_m = \frac{k_f}{B} + \frac{v}{aL} \ln \left\{ \frac{B + \frac{D'}{B^2} (1 - B) \exp \left[-\alpha L \left(\frac{1}{B} + \frac{B}{D'} \right) \right]}{1 + D'/B^2} \right\} \quad (4)$$

where

$$\begin{aligned} \alpha &= ak_f/v \\ D' &= \epsilon ak_f E/v^2 \\ B &= \frac{1 + \sqrt{1 + 4D'}}{2} \end{aligned}$$

The boundary conditions used to solve equation 3 were those given by Wehner and Wilhelm's analysis (36).

$$vc_F = - E \frac{dc}{dz} + vc \quad \text{at} \quad z = 0 \quad (5i)$$

$$\frac{dc}{dz} = 0 \quad \text{at} \quad z = L \quad (5ii)$$

Equation 4 shows how the experimentally accessible, and design useful, k_m can be corrected to give the film coefficient k_f . For purely pedagogical purposes, assume k_f is given by the Wilson-Geankopolis correlation (34). Figure 1 (26) illustrates how k_m would then vary with the Péclet number. At large Péclet numbers, the distinction between the two coefficients vanishes. However, as $Pe_B \rightarrow 0$, the difference between the two becomes important. It should perhaps be emphasized that the calculation of k_f from k_m requires a value of E , with which there must be associated some uncertainty.

Calculation of k_m

It would not be necessary to use the one-dimensional model for a bed and its associated film coefficient if we could describe the void volume in the bed analytically. For it would then be possible (in principle) to solve the hydrodynamics and the convective-diffusion within the voids to calculate directly the overall conversion. This is an overwhelming task. The voids in a bed defy

an analytic expression except in simple instance (34). This approach, however, can be used to indicate the asymptotic behavior of the fluid-to-particle transfer rate at low Péclet numbers. We shall see that a detailed knowledge of the void volume function is not necessary to establish the behavior in this limit.

Assuming a known bed geometry, we shall demonstrate how k_m (not k_f) behaves asymptotically as $Pe_B \rightarrow 0$. Equation 4 with the proper form of the dispersion coefficient can then be used to indicate the behavior of k_f .

Wehner and Wilhelm (36) showed how to analyze correctly the behavior of a one-dimensional model for a packed bed reactor. Their analysis can be extended to the actual three-dimensional structure of the bed. As shown in figure 2, the bed consists of three regions. Region II of length L is the reactive section of the bed. Regions I and III extend in the dimensionless streamwise coordinate x_1 to $-\infty$ and $+\infty$, respectively. They are filled with an inert packing. These are the "calming sections" used in experimental apparatus. A cross section normal to the streamwise direction is finite in extent.

The position of the particles' surface is assumed to be known as a function of the streamwise coordinate. Designate this function as $W_a(x_1)$ for the reactive particles and $W_i(x_1)$ for all other inactive surfaces.

Neglecting free convection effects, the concentration field in the voids will satisfy the dimensionless convective-diffusion equation.

$$\vec{v} \cdot \nabla c/c_F = \frac{1}{Pe_B} \nabla^2 c/c_F \quad (6)$$

Equation 6 is subject to the following boundary conditions.

$$\begin{aligned} \text{i)} \quad x_1 \rightarrow -\infty \quad & \frac{c}{c_F} = 1 \\ \text{ii)} \quad -\infty < x_1 < \infty \quad & \frac{\partial(c/c_F)}{\partial n} = 0 \quad \text{on } W_i(x_1) \\ \text{iii)} \quad 0 \leq x_1 \leq aL \quad & \frac{c}{c_F} = 0 \quad \text{on } W_a(x_1) \\ \text{iv)} \quad x_1 \rightarrow \infty \quad & \frac{c}{c_F} \text{ remains finite.} \end{aligned} \quad (7)$$

These boundary condition yield a well-posed problem when applied to equation 6 in the void volume.

Equation 7(iv) is a valid constraint placed on the solution. An auxiliary condition can also be written for the far downstream concentration field.

$$\frac{c}{c_F} (x_1 \rightarrow \infty) = e^{-\beta L} \quad (8)$$

Here βL is some unknown constant which must be determined as part of the solution. This parameter is directly related to the effective mass-transfer coefficient k_m as can be seen from equating equations 8 and 2.

$$\text{Sh}_B = \text{Pe}_B \frac{\epsilon}{aL} \beta L. \quad (9)$$

As expected, we see that the solution to the detailed convective-diffusion equation yields the effective coefficient directly. In the most general situation, βL will be a function of the velocity field, the parameters Pe_B and aL , and the geometric functions $W_i(x_1)$ and $W_a(x_1)$.

We want to consider the solution to equations 6 and 7 in the limit of zero Péclet number. This limiting process is singular in nature. There are regions in the bed where diffusion does not dominate the reactant transport and convection becomes important. These regions will be located in the upstream and downstream "calming" sections. There are precedents for this expected behavior in the literature. Acrivos and Taylor (1) analyzed a single reactive sphere in Stokes flow as the particle Péclet number approaches zero. They have shown that, near the sphere, diffusion controls the mass-transfer rate to the surface, but convection also becomes important far from the surface. Leal (15) has extended this analysis to a sphere in a simple shear field. Such work suggests that applying the asymptotic limit of $\text{Pe}_B \rightarrow 0$ will require a singular perturbation approach.

To formulate properly a singular perturbation problem for the concentration field within the voids of the bed, it is necessary to delineate the regions where diffusive and/or convective transport are controlling. Appropriate transformation variables must also be defined for each region. The equations governing the concentration

and their boundary conditions should then be independent of the Péclet number in the regions.

In the reactor section (II) and a region on the "calming" side of the boundaries I-II and II-III, the inner solution applies. In the inner expansion, diffusion dominates the reactant transport. Far away from the reactor section, in the upstream (I) and downstream (III) regions, the diffusive and convective flux of reactant become equally important. Thus, there is an upstream and downstream outer region to the expansion.

Consideration of the Wehner-Wilhelm solution for a one-dimensional bed leads to the appropriate transformed concentration and coordinates in each region.

$$\begin{aligned} \tilde{\theta}^I &= c/c_F \\ \tilde{x}_j^I &= x_j \frac{Pe_B}{\epsilon} \quad (j = 1, 2, 3) \end{aligned} \left. \vphantom{\begin{aligned} \tilde{\theta}^I \\ \tilde{x}_j^I \end{aligned}} \right\} \begin{array}{l} \text{upstream} \\ \text{outer} \\ \text{variables} \end{array}$$

$$\begin{aligned} \bar{\theta} &= \frac{c\epsilon}{c_F Pe_B} \\ \bar{x}_j &= x_j \quad (j = 1, 2, 3) \end{aligned} \left. \vphantom{\begin{aligned} \bar{\theta} \\ \bar{x}_j \end{aligned}} \right\} \begin{array}{l} \text{inner} \\ \text{variables} \end{array}$$

$$\begin{aligned} \tilde{\theta}^{III} &= \frac{c\epsilon}{c_F Pe_B} \\ \tilde{x}_j^{III} &= (x_j - aL\delta_{1j}) \frac{Pe_B}{\epsilon} \quad (j = 1, 2, 3) \end{aligned} \left. \vphantom{\begin{aligned} \tilde{\theta}^{III} \\ \tilde{x}_j^{III} \end{aligned}} \right\} \begin{array}{l} \text{downstream} \\ \text{outer} \\ \text{variables} \end{array}$$

The coordinates (x_1, x_2, x_3) form an orthogonal system with its origin at the geometric center of the entrance to section II. Coordinate x_1 is in the streamwise direction. The tilde (\sim) refers to the outer region variables and the bar ($\bar{}$) refers to inner region variables. The transformed concentrations have been scaled to be of $O(1)$ in each region.

In the upstream and downstream outer region expansion, further simplifications are possible. Far from the perturbing effect of the reactor section, the concentration field will be approaching a constant value at each cross section of the bed, that is, the variation in the axial direction is small over a distance comparable to the size of a particle. Thus the one-dimensional (streamwise) description will suffice as a first-order approximation. The geometry is a second-order effect there. It is accounted for by the tortuosity factor in the effective diffusion coefficient. In the inner region of the expansion, however, the exact placement of the particles is important, and no geometrical simplifications can be made here.

By the above reasoning, the first-order solution in each region is governed by the following equations.

$$\frac{d^2 \tilde{\theta}_o^I}{d(\tilde{x}_1^I)^2} - \frac{d\tilde{\theta}_o^I}{d(\tilde{x}_1^I)} = 0 \quad (10)$$

$$\nabla^2 \bar{\theta}_o = 0 \quad (11)$$

$$\frac{d^2 \tilde{\theta}_o^{\text{III}}}{d(\tilde{x}_1^{\text{III}})^2} - \frac{d \tilde{\theta}_o^{\text{III}}}{d(\tilde{x}_1^{\text{III}})} = 0 \quad (12)$$

Equation 10 is subject to the boundary condition 7(i) and equation 12 to 7(iv). Equation (11) is subject to equations 7(ii), 7(iii), and the matching condition imposed by merging the outer limit of the inner solution to the inner limit of the outer solution. This is carried out in the upstream and downstream regions. This matching results in the following additional boundary conditions for equation (11).

$$\frac{\partial \bar{\theta}_o}{\partial \bar{x}_1} = -1 \quad \text{as} \quad \bar{x}_1 \rightarrow -\infty \quad (13)$$

$$\frac{\partial \bar{\theta}_o}{\partial \bar{x}_1} = 0 \quad \text{as} \quad \bar{x}_1 \rightarrow \infty .$$

The first order governing equations and their necessary boundary and matching conditions have been outlined above. The solution to this system of equations then generates the first-order approximation to the concentration of the reactant leaving the bed. This result can be utilized in equations 8 and 9 to write,

$$\frac{\epsilon k_m}{aD_o} = \frac{\epsilon}{aL} \frac{v}{aD_o} \left[\ln 1/\theta_L - \ln \frac{v}{\epsilon a D_o} \right] \quad (14)$$

where θ_L is $\lim_{\bar{x}_1 \rightarrow \infty} \bar{\theta}_0$. Equation 14 has been rigorously derived through a singular perturbation approach. The bed Sherwood number for low Péclet numbers can be calculated once θ_L is known. This quantity will depend upon the detailed geometry functions W_i and W_a , and the parameter aL , as can be seen by examining equations 10 through 12 and their associated boundary conditions.

Equation 14 may appear to be a rearrangement of equation 1, and indeed it can be generated from equation 1 through algebraic manipulations. However, equation 14 yields a priori predictions of the Sherwood number after θ_L is determined from the perturbation problem as outlined. In particular, θ_L is shown to be independent of the Péclet number at low Péclet numbers, and the dependence on aL can be elucidated to some extent as discussed below.

Deep bed behavior of k_m

For straight tubes with an insulated upstream wall ($z < 0$) and an active downstream wall ($z \geq 0$), the local mass-transfer rate depends upon the axial position, but the local mass-transfer coefficient approaches an asymptotic value in the downstream region. The length scale in which this asymptotic value is approached depends upon the Péclet number. This region is usually designated the mass-transfer entry region. Levich (16) has shown for high Péclet numbers that the entry region is $O(\text{Pe}R)$, where R is the tube radius. In the low Péclet number regime, Michelsen and Villadsen (18) have shown that the entry region is $O(R)$, a result which is substantiated by

the calculations of Sørensen and Stewart (33) and Michelsen and Villadsen (18).

From these results one concludes that the entry region for a packed bed should be in the order of a particle diameter for low Péclet numbers, and a deep bed thus will be one for which $L \gg d_p$. In this limit, most of the bed will be in the well-developed mass-transfer region, where the fractional decrease of reactant for any incremental streamwise length should be independent of the position of the incremental length. Thus, for deep beds, the dependence of θ_L on aL can be expressed as

$$\theta_L = \alpha_2 e^{-\alpha_1 aL/\epsilon} \quad , \quad (15)$$

where α_1 and α_2 are independent of aL (as well as Pe) and are dependent upon the detailed geometric functions W_i and W_a . The deep bed, low Pe_B Sherwood number from equation 14 can then be written as

$$\frac{\epsilon k_m}{aD_o} = \frac{v}{aD_o} \left[\alpha_1 - \frac{\epsilon}{aL} \ln \frac{\alpha_2 v}{\epsilon a D_o} \right] \quad . \quad (16)$$

Since the entry region is small at low Péclet numbers, this result should be applicable to many beds of practical importance. Equation 16 was first stated by Sørensen and Stewart (34) but they did not demonstrate how they derived this result.

Equation 16 shows that for large values of aL , where the second term in the brackets is negligible compared to the first, k_m becomes linearly proportional to the velocity. (Note that in figure 1 the curve for $aL = 5$ is fairly close to that for $aL = \infty$.) After applying the large aL limit and the low Péclet number limit, one can conclude from equation 4 that the film coefficient of the one-dimensional model for the same bed must approach a constant as

$$\frac{\epsilon k_f}{aD_o} = \alpha_1^2 \frac{\epsilon}{\tau} \quad (17)$$

Equations 16 and 17 are the main result of this paper. It is worth noting that equation 16 could be derived from equation 4 in a simpler manner by a priori postulating that k_f becomes independent of v for low Péclet numbers. However, this of course would not shed any conclusive light on the real behavior of k_f .

The void volume approach outlined above cannot be carried further for the general case without specifying the geometry. A packed bed can be considered on the microscopic scale as a statistically periodic structure (27). In order to introduce a predictive capability into the present method, one can solve equation 11 in the well-developed mass-transfer region as an eigenvalue problem. This yields the fractional decrease of reactant for each period and hence the value of α_1 in equation 15. For significant values of aL , this also yields the dominant part of k_m according to equation 16 and k_f according to equation 17.

Discussion

The two types of mass-transfer coefficients described in this work have been reported in the literature. Miyauchi and his co-authors (20,21,22,23) conclude from the analysis of their data that the film coefficient reaches a constant as the Péclet number decreases. Gunn and Souza (10) and Littman *et al.* (17) also reach the same conclusion about their data. However, their results exhibit more scatter than those of Miyauchi. On the other hand, from considering those workers' results (3,6,7,9,13,25,28,31) who calculated an effective transfer coefficient as in equation 1 (or its possible equivalent forms), one could conclude that the effective transfer coefficient decreases with decreasing Péclet number.

There are clearly different experimental trends in these two coefficients. Our analysis suggest that the effective Sherwood number becomes linearly proportional to the Péclet number as $Pe \rightarrow 0$. This is true for any geometric arrangement of the voids in the bed. This implies through equation 4 that the film coefficient approaches a constant in the same limit. These predicted trends agree with the available experimental data.

We have not been concerned in this paper with presenting numerical predictions for the film or effective mass-transfer coefficients at low Péclet numbers. However, several comments on some previous theoretical work along this line are in order.

To predict the transfer coefficients in a bed, it is necessary to introduce a microscopic model for the structure of the bed. The

free-surface cell model developed by Happel (11) or an analog of this as introduced by Neal and Nader (24) has been used by various authors. One can calculate a film mass-transfer coefficient by solving the hydrodynamics and the convective-diffusion equation within the cell, both subject to appropriate boundary conditions. This film coefficient will depend upon the flow conditions in the cell and the Schmidt number. As our analysis suggests, only in the high Péclet number region is this film coefficient equal to the effective coefficient k_m . Pfeffer (29), Pfeffer and Happel (30), El-Kaissy and Homsy (8) and Tardos *et al.* (35), have performed such calculations for high Péclet numbers within the free-surface cell model framework.

At low Péclet numbers, the uniform concentration boundary condition imposed on the outer free surface of the cell has been criticized (5,25,33). Nelson and Galloway (25) attempted to remedy this fictitious sink boundary condition. They imposed a zero-radial gradient condition on the concentration at the outer free surface. They combined surface-renewal and boundary-layer arguments to arrive at a film coefficient linearly proportional to the Reynolds number and to the Schmidt number raised to the two-thirds power. At low Reynolds numbers the applicability of surface-renewal theory and boundary-layer theory is questionable. Also, the distinction between the film and effective mass-transfer coefficients was not recognized.

Kunii and Susuzikki (14) have realized the difference between the two coefficients at low Péclet numbers. They have presented

a channeling model to calculate k_m . They predict a linear dependence on the Péclet number. Their model involves an empirical factor which varies over two orders of magnitude to fit their data analysis.

Sørensen and Stewart (34) have numerically calculated the creeping flow velocity profiles and solved the convective-diffusion equation for a limiting reactant in a simple cubic packed bed of uniform sized spheres. These calculations are a great aid in the understanding of processes in an actual bed. Their results indicate that the effective coefficient k_m varies linearly with the Péclet number as $Pe_B \rightarrow 0$ in accord with equation 16. Their results can be used to calculate α_1 in equation 16, and hence, through equation 17, k_f . The dimensionless film coefficient for a deep bed of simple-cubic packed spheres ($\epsilon \sim 0.48$) is found to be

$$\frac{d k_f}{D_0} = 3.4$$

where a tortuosity factor of $\tau = \sqrt{2}$ has been assumed. This should be compared to the experimental values of 12.5 determined by Miyauchi et al. (19) for a gas-film coefficient ($\epsilon \sim 0.5$), of 16.7 determined by Miyauchi et al. (20) for a liquid-film coefficient ($\epsilon \sim 0.4$), and of 10.0 determined by Gunn and Souza (9) for a gas film coefficient ($\epsilon \sim 0.4$).

It should be noted that Sørensen and Stewart's results have been previously misunderstood. Their calculations do not imply a dimensionless film coefficient of 3.9 as has been claimed. Their Nusslet

number Nu is based on the log mean average of the convective energy flux entering and leaving the bed. This number is not the low Péclet number, one-dimensional film coefficient.

Summary

It has been demonstrated that the low Péclet number behavior of the Sherwood number in a packed bed reactor is dependent upon its defining equation. A rigorous singular perturbation approach coupled with heuristic arguments indicates that for a deep bed the effective mass-transfer coefficient (defined by equation 1) is directly proportional to the Péclet number. The film coefficient (defined by equation 3) approaches a constant in the same limit. These conclusions are independent of the detailed geometric void structure in the bed.

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Nomenclature

a	specific interfacial area, cm^{-1}
c_F	far upstream reactant concentration, mol/cm^3
c_L	far downstream reactant concentration, mol/cm^3
D_o	molecular diffusion coefficient, cm^2/s
E	dispersion coefficient, cm^2/s
k_f	film mass-transfer coefficient, equation 3, cm/s
k_m	effective bed mass-transfer coefficient, equation 1, cm/s
L	reaction section length, cm
n	normal coordinate, cm
Pe_B	bed Péclet number $\frac{v}{aD_o}$
Sh_B	bed Sherwood number, $\frac{\epsilon k_m}{aD_o}$
v	superficial velocity, cm/s
x_1, x_2, x_3	dimensionless bed coordinates, ax_d
z	streamwise dimensional coordinate
Creek	
δ_{ij}	Kronecker delta
ϵ	porosity
τ	tortuosity
Subscripts	
d	dimensional quantity
ln	logarithmic mean

References

1. Acrivos, A., and T. O. Taylor, Phys. Fluids, 1962, 5, 387.
2. Appel, P. W., and J. Newman, AIChE J. 1976, 6, 979.
3. Bar-Ilan, M., and W. Resnick, Ind. Eng. Chem., 1957, 49, 313.
4. Bird, R. B., W. E. Stewart, and E. N. Lightfoot, Transport Phenomena, 1960, pp. 390-396.
5. Cornish, A. R., Trans. Instn. Chem. Eng., 1965, 43, 7332.
6. Dryden, C. E., Chem. Eng. Prog., 1953, 49, 191.
7. Eichorn, J., and R. R. White, Chem. Eng. Prog. Symp. Ser., 1952, 48, 11.
8. El-Kaissy, M., and G. M. Homsy, IEC Fund., 1973, 12, 82.
9. Gliddon, B. J., and R. R. Cramefield, Brit. Chem. Eng., 1970, 15, 489.
10. Gunn, D. J., and J. F. C. De Souza, Chem. Eng. Sci., 1974, 29, 1363.
11. Happel, J., AIChE J., 1958, 4, 197.
12. Karabelas, A. J., T. H. Wagner, and T. H. Hanratty, Chem. Eng. Sci., 1971, 26, 1581.
13. Kato, K., H. Kubota, and C. W. Yen, Chem. Eng. Prog. Symp. Ser., 1970, 66, 87.
14. Kunni, D., and M. Suzuki, Int. J. Heat Mass Transfer, 1967, 10, 845.
15. Leal, L. G., Chem. Eng. Commun., 1973, 1, 21.
16. Levich, V. G., Physicochemical Hydrodynamics, 1962, Prentice-Hall, p. 113.

17. Littman, H., R. G. Barile, and A. H. Pulsifer, IEC Fund., 1968, 7, 554.
18. Michelsen, M. L., and J. Villadsen, Int. Heat Mass Transfer, 1974, 17, 1391.
19. Miyauchi, T., J. Chem. Eng. Japan, 1971, 4, 238.
20. Miyauchi, T., T. Kikuchi, and H. Kataoka, Int. Chem. Eng., 1972, 12, 373.
21. Miyauchi, T., K. Matsumoto, and T. Yoshida, J. Chem. Eng. Japan, 1975, 8, 228.
22. Miyauchi, T., H. Kataoka, and T. Kikuchi, Chem. Eng. Sci., 1976a 31, 9.
23. Miyauchi, T., T. Kikuchi, and K. H. Hsu, Chem. Sci., 1976b 31, 493.
24. Neal, G. H., and W. K. Nader, AIChE J., 1973, 19, 112.
25. Nelson, P. A., and T. R. Galloway, Chem. Eng. Sci., 1975, 30, 1.
26. Newman, J., and W. Tiedemann, 1977, in press, Advances in Electrochemistry and Electrochemical Engineering.
27. Payatakes, A. C., C. Tien, and R. M. Turian, AIChE J., 1973, 19, 58.
28. Petrovic, L. J., and G. T. Thodos, IEC Fund., 1968, 7, 274.
29. Pfeffer, R., IEC Fund., 1964, 3, 383.
30. Pfeffer, R., and J. Happel, AIChE J., 1964, 10, 605.
31. Resnick, W., and R. R. White, Chem. Eng. Prog., 1949, 45, 377.
32. Sherwood, T. R., R. L. Pigford, and C. R. Wilke, Mass Transfer, 1975, p. 43 and p. 129.
33. Sorenson, J. P., and W. E. Stewart, Chem. Eng. Sci., 1974, 29, 811.

34. Sørensen , J. P., and W. E. Stewart, Chem. Eng. Sci., 1974, 29, 827.
35. Tardos, G. I., C. Gutfinger, and N. Abuaf, AIChE J., 1976, 22, 1147.
36. Wehner, J. F., and R. H. Wilhelm, Chem. Eng. Sci., 1956, 6, 89.
37. Wilson, E. J., and C. J. Geankopolis, IEC Fund., 1966, 5, 9.

Table I: Compilation of works which have reported heat or mass transfer data in packed beds for a particle Péclet number less than 30.

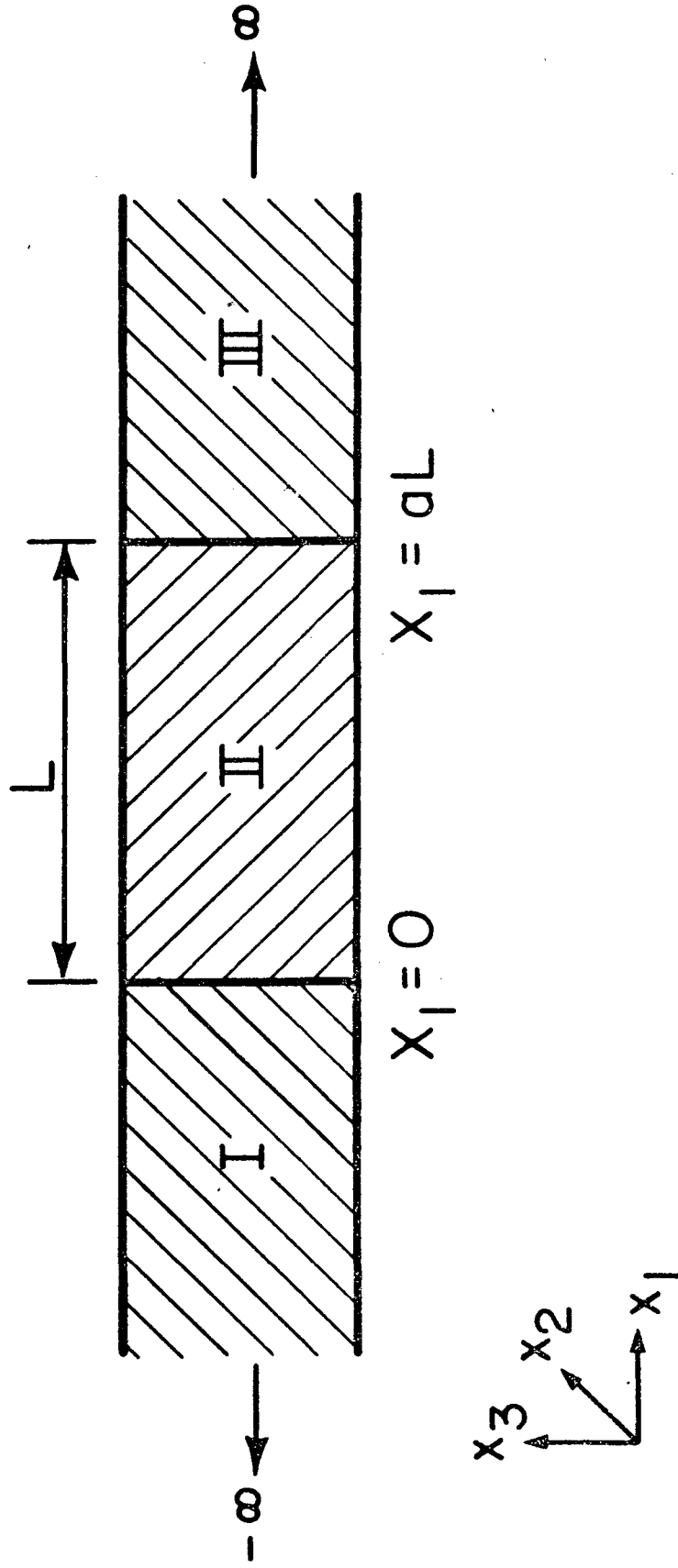
Investigators	Lowest Reynolds number reported	Lowest Schmidt or Prandtl number reported	Lowest Péclet number	Heat (H) or Mass (M)
Resnick and White (1949)	0.62	4.0	2.5	M
Eichorn and White (1952)	1	0.7*	0.7	M
Dryden <u>et al.</u> (1953)	0.0125	814	10.2	M
Bar-Ilan and Resnick (1957)	0.2	2.6	0.5	M
Littman <u>et al.</u> (1968)	1.9	0.7*	1.3	H
Petrovic and Thodos (1968)	3	0.6	1.8	M
Kato, <u>et al.</u> (1970)	0.1	2.6	0.3	M
Gliddon and Cranefield (1970)	23.8	0.7	16.4	H
Karabelas <u>et al.</u> (1971)	0.01	1490	15	M
Gunn and De Souza (1974)	1.5	0.7*	1.1	H
Miyauchi <u>et al.</u> (1975)	0.02	510	10	M
Nelson and Galloway (1975)	1	0.7*	0.7	H
Miyauchi <u>et al.</u> (1976a)	?	?	2	M
Appel and Newman (1976)	0.00806	1440	11.6	M

* estimated value

Figure Captions

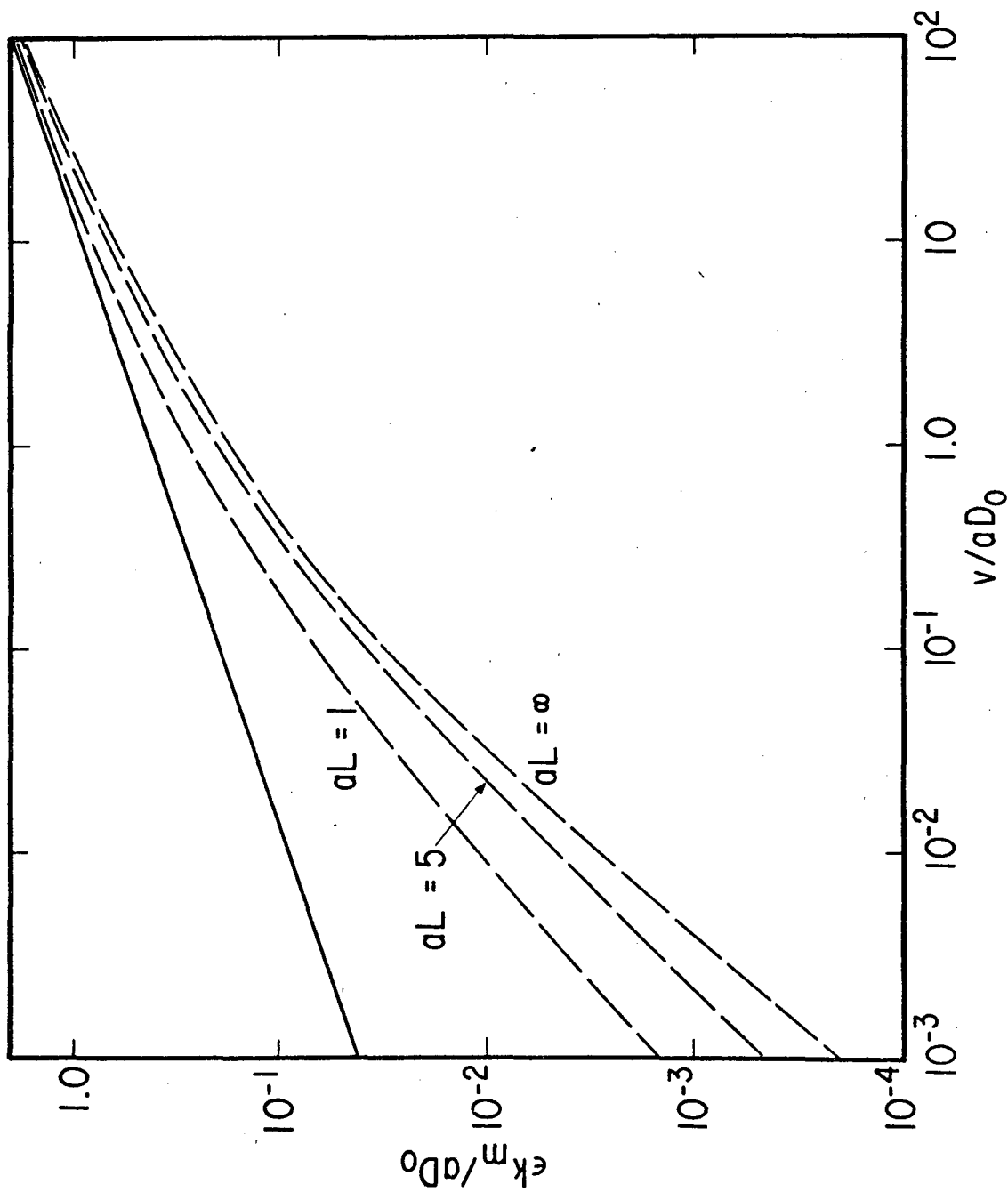
Figure 1 Influence of axial dispersion on the effective mass-transfer coefficient k_m . The film mass-transfer coefficient k_f is assumed to be given by the Wilson-Geankopolis correlation (37) as shown in the upper curve. Because of axial dispersion, k_m lies below k_f , and the effect becomes large at low Péclet numbers. In preparing the graph, the porosity was taken to be $\epsilon = 0.3$ and the tortuosity factor τ was assumed to be 1. The convective contribution to the dispersion coefficient was given by equation 14 of reference 26.

Figure 2 Schematic of a packed bed with fore and aft "calming" sections.



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Figure 1.



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Figure 2.

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