Accuracy of the Axial Dispersion Model for Chemical Reactors

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The axial dispersion model has been extensively used to represent mixing effects in chemical reactors (*3, 8*). Since this model gives only, in some sense, a cross section averaged description of the reactor, there is a question concerning its ability to represent adequately the actual two-dimensional phenomena occurring. One way to check this, of course, is to compare experimental reactor data with the model predictions (*9*). As a final test this is probably the best, but because of the many experimental problems in kinetics, it is difficult to get very high precision. In other words, it is often difficult to decide whether any discrepancies are from the model or the data. Thus, it would seem that a mathematical comparison between the axial dispersion model and the more precise two-dimensional calculations would be useful.

This has been done for the problem of dispersal of matter in the classic papers of Taylor (*11, 12*) with extensions by Aris (*2*), and Gill, et al. (*1, 6, 10*). However, the results and criteria are not really definitive for the actual problem of chemical reactors since the physical nature is somewhat different. A direct comparison for the case of a first-order reaction with laminar flow can be easily accomplished since the axial dispersion model solution has been given by Wehner and Wilhelm (*13*) and the two-dimensional solution by Cleland and Wilhelm (*5*), Lauwerier (*7*), and Wissler and Schechter (*14*).

Before proceeding to the mathematical details, it might be useful to consider the qualitative results to be expected. The classical Taylor-Aris formulation requires the stipulation that a long system be considered. In other words, a certain time must elapse after the introduction of the solute before the dispersion process can be represented by a one-dimensional treatment. This treatment has been extended to include a first-order reaction by Bischoff and Levenspiel (*4*), but here some reaction time constant must also be long compared with the residence time, if the axial dispersion model is to be valid. This means that the reaction must be relatively slow so that sufficient time can elapse as in the Taylor-Aris criterion. Thus, it would seem that the axial dispersion model would be most accurate for a slow reaction occurring in a long reactor. The exact meaning of these qualifications, however, must be found from the mathematical equations.

ANALYSIS

The two-dimensional mass balance representing diffusion in symmetric laminar flow in a round tube with a first-order chemical reaction is (*7, 14*)

$$2v\left(1-\frac{r^2}{R^2}\right)\frac{\partial C}{\partial z}=\frac{\mathcal{D}}{r}\frac{\partial}{\partial r}r\frac{\partial C}{\partial r}+\mathcal{D}\frac{\partial^2 C}{\partial z^2}-kC \tag{1}$$

If Equation (1) is made dimensionless as done by Lauwerier, Wissler, and Schechter, the result is

$$4(1-r^{+2})\frac{\partial C^+}{\partial z^+}=\frac{1}{r^+}\frac{\partial}{\partial r^+}r^+\frac{\partial C^+}{\partial r^+}+4\left(\frac{\mathcal{D}}{vR}\right)^2\frac{\partial^2 C^+}{\partial z^{+2}}-4\alpha C^+ \tag{2}$$

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The cross section flow mean concentration at the reactor exit is what is desired for the comparison, and this is

$$\overline{C_L{}^+}=4\int_0^1 r^+(1-r^{+2})\,C_L{}^+\,dr^+ \tag{3}$$

The statement of the axial dispersion model for the same problem is (*13*)

$$v\frac{dC}{dz}=D_L\frac{d^2C}{dz^2}-kC \tag{4}$$

If the same dimensionless variables are used, then

$$2\frac{dC'}{dz^+}=4\left(\frac{D_L}{vR}\right)\left(\frac{\mathcal{D}}{vR}\right)\frac{d^2C'}{dz^{+2}}-4\alpha C' \tag{5}$$

where $C'=C/C_o$ is used to denote the concentration from the axial dispersion model.

Now the comparison between the two models will be made by substituting the Taylor-Aris formula for D_L in terms of $\mathcal{D}$, v, and R into Equation (5) and comparing its solution with that of Equations (2) and (3). Actually, Lauwerier (*7*), and Wissler and Schechter (*14*) only solved the case where axial molecular diffusion was negligible. This means that the second derivative in z term in Equation (2) was neglected. Thus, to be consistent, the original Taylor expression, which also neglected axial molecular diffusion, must be used rather than the complete Aris expression:

$$D_L=\frac{1}{48}\frac{v^2R^2}{\mathcal{D}^2} \tag{6}$$

The solution of Wehner and Wilhelm (*13*) for Equation (5) at the reactor exit was given as

$$C_L{}'=\frac{4a\exp\left(\frac{1}{2}N_{Pe}\right)}{(1+a)^2\exp\left(\frac{a}{2}N_{Pe}\right)-(1-a)^2\exp\left(\frac{a}{2}N_{Pe}\right)} \tag{7}$$

Lauwerier (*7*), and Wissler and Schechter (*14*) used an eigenfunction expansion technique, which gave the same results as the finite difference calculations of Cleland and Wilhelm (*5*), and their results for the cross section average could be expressed as

$$\overline{C_L{}^+}=4\sum_{n=1}^{\infty}A_n{}^2\,N_n\,e^{-\omega_n z_L{}^+} \tag{8}$$

where the numerical values of $\omega_n(\alpha)$, $A_n(\alpha)$ and $N_n(\alpha)$ have been tabulated by Wissler and Schechter (*14*). The values of $C_L{}^+$ from Equation (8) can now be compared with those of $C_L{}'$ from Equation (7) for corresponding values of $z_L{}^+$ and α.

NUMERICAL RESULTS

The numerical results computed from Equations (7) and (8) are shown in Table 1. It is seen that for a fairly slow reaction (small $\alpha = 0.25$), the agreement between the axial dispersion model and the two-dimensional calculations is essentially perfect. For faster reaction rates

(larger $\alpha = 2.5$), the comparison is still good, but for high reaction rates ($\alpha = 25$), large deviations begin to occur. These results are more or less as expected from the discussion above, but now give more quantitative criteria. It is seen that over a rather wide practical range of the parameters, the axial dispersion model provides a good approximation to the more exact, but more complicated, three-dimensional equations. Since laminar flow is an extreme example of sharp velocity profile, the use of the axial dispersion model for other cases, such as turbulent flow with a more flat velocity profile, should be satisfactory.

TABLE 1.

z_L^+	$\overline{C_L}^+$	C_L'	N_{Pe}	R_1
$\alpha = 0.25$				
0.2	0.906	0.907	4.8	0.1
0.4	0.821	0.822	9.6	0.2
0.6	0.744	0.745	14.4	0.3
0.8	0.675	0.676	19.2	0.4
1.0	0.612	0.612	24.0	0.5
$\alpha = 2.5$				
0.2	0.405	0.417	4.8	1.0
0.6	0.073	0.076	14.4	3.0
1.0	0.0135	0.0140	24.0	5.0
$\alpha = 25$				
0.02	0.421	0.455	0.48	1.0
0.05	0.144	0.218	1.2	2.5
0.10	0.028	0.064	2.4	5.0

Recently, Horn and Parish (*15*) have presented a theoretical justification of the use of the axial dispersion model similar to the analysis of Taylor and Aris, but actual numerical criteria were not given.

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NOTATION

a = parameter $= \sqrt{1 + 4R_1/Bo} = \sqrt{1 + \alpha/3}$
A_n = constant in eigenvalue expansion, Equation (8)
C = concentration
C_o = feed concentration
C^+ = dimensionless concentration $= C/C_o$
$\overline{C_L}^+$ = cross section flow mean concentration at reactor exit, defined by Equation (3)
C' = dimensionless mean concentration found from axial dispersion model
$\mathcal{D}$ = molecular diffusivity
D_L = axial dispersion coefficient
k = reaction rate coefficient
N_n = constant in mean concentration expansion, Equation (8)
N_{Pe} = dimensionless Peclet number $= vz_L/D_L$
r = radial coordinate
r^+ = dimensionless radial coordinate $= r/R$
R = tube radius
R_1 = rate group $= kz_L/v$
v = mean velocity
z = axial coordinate
z_L = reactor length
z_L^+ = dimensionless reactor length $= 2\mathcal{D}z_L/vR^2 = N_{Pe}/24$
α = parameter $= kR^2/4\mathcal{D}$
ω_n = eigenvalue

Superscripts

$+$ = dimensionless variable
= refers to axial dispersion model concentration

Subscript

L = refers to value at end of reactor

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Methods of Predicting the Occurrence and Type of Fluid-Fluid Equilibria in Binary Systems

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In a recent paper (*1*) I presented a semiempirical method (the D^2 method) by which gas-gas equilibrium (limited mutual solubility of gases at temperatures above the critical temperature of the least volatile component) could be predicted for binary systems on the basis of critical data and experimental gas-gas equilibria results on systems not necessarily containing either of the components of the system whose behavior is in question.

The types of gas-gas equilibrium are designated as type I or II, depending on whether the $p(T)$ critical curve, starting from the critical point of the least volatile component, has a positive or negative slope. Figure 1 shows the difference between these two types and usual critical curve behavior. The one shortcoming of the D^2 method is that it does not predict what type of gas-gas equilibrium will occur. Another simple method that is in good agreement