E = activation energy
$(-\Delta H)$ = exothermic heat of reaction
k_o = frequency factor
q = volumetric flow rate
R = gas constant
T = temperature
$\overline{T}$ = dimensionless temperature, see Equation (3)
T_c = coolant temperature
T_i = initial dimensionless temperature
T_o = inlet temperature
U = overall heat transfer coefficient
V = reactor volume

Greek Letters

α see Equation (8)
β see Equation (9)
γ see Equation (10)
δ see Equation (11)
ρ = density of reactor contents
θ = time
$\overline{\theta}$ = dimensionless time, see Equation (5)

LITERATURE CITED

1. Bilous, Olegh, and N. R. Amundson, *A.I.Ch.E. J.*, **1**, 513 (1955).
2. Berger, J. S., and D. D. Perlmutter, *ibid.*, **10**, 233 (1964).
3. ———, *Chem. Eng. Sci.*, **20**, 147 (1965).
4. Paradis, W. O., and D. D. Perlmutter, *A.I.Ch.E. J.*, **12**, 130 (1966).

Effective Dispersion in a Tubular Flow Reactor with Return Bends

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The characterization of nonideal flow conditions in chemical reactors has received considerable attention recently, and is a logical step to be taken toward the realization of a closer design of chemical reactors. In the case of tubular reactors, or those that approach plug flow conditions, the use of a dispersion coefficient to take into account local mixing, as well as radial velocity variations, seems to be practical (*3, 4*). In the case of reactors with configurations that disrupt or bypass the flow, the use of mixed models has been proposed (*3, 4*). Bischoff (*1*) recently worked with a mixed model to obtain an effective dispersion coefficient from the data of Carter and Bir (2) on axial mixing in a tubular reactor with a number of return bends. He considered the straight sections as plug flow sections with axial mixing, and the return bends as perfect mixers. The representation of the return bends as completely mixed sections gives effective dispersion coefficients that fit the experimental data better than if the bends are ignored. A better fit might be expected if the return bends are considered as sections of greater axial mixing than the straight sections, but not as perfect mixers. We would like to illustrate this point by the use of a dispersion model where the dispersion coefficient for the return bends is a function of the dispersion coefficient in the straight sections and Reynolds number. The effective dispersion can then be made to exhibit a minimum as the Reynolds number is increased.

MODEL

Suppose we consider the dispersion coefficient at the bend section as some multiple of the dispersion coefficient in a straight pipe, that is

$$D_b = m\, D_p \tag{1}$$

This implies that the dispersion group at the bend section is

$$\frac{D_b}{v\, L_{\text{beq}}} = m \frac{D_p}{v\, L_{\text{beq}}} \tag{2}$$

where L_{beq} is an equivalent length of the bend section. Then in a treatment similar to Bischoff's (*1*), the first and second moments for the straight sections are

$$\Delta\mu_{1p} = \left(\frac{L_p}{L}\right) \tag{3}$$

$$\Delta\sigma^2{}_p = 2\frac{D_p}{v\, L_p}\left(\frac{L_p}{L}\right)^2 \tag{4}$$

for the bend sections

$$\Delta\mu_{1b} = \left(\frac{L_{\text{beq}}}{L}\right) \tag{5}$$

$$\Delta\sigma_b{}^2 = m^2\, \Delta\sigma^2{}_{\text{peq}} = m^2\left(2\frac{D_p}{v\, L_{\text{beq}}}\right)\left(\frac{L_{\text{beq}}}{L}\right)^2 \tag{6}$$

and for the overall system

$$\Delta\mu_1 = 1 \tag{7}$$

$$\Delta\sigma^2 = 2\left(\frac{D_e}{v\, L}\right) \tag{8}$$

From Equations (4), (6), and (8)

$$\frac{De}{v\, L} = \frac{Dp}{v\, L}\left(\frac{Lp}{L}\right) + m^2\frac{Dp}{v\, L}\left(\frac{L_{\text{beq}}}{L}\right) \tag{9}$$

But from Equations (3), (5), and (7)

$$\frac{L_p}{L} = 1 - \left(\frac{L_{\text{beq}}}{L}\right) \tag{10}$$

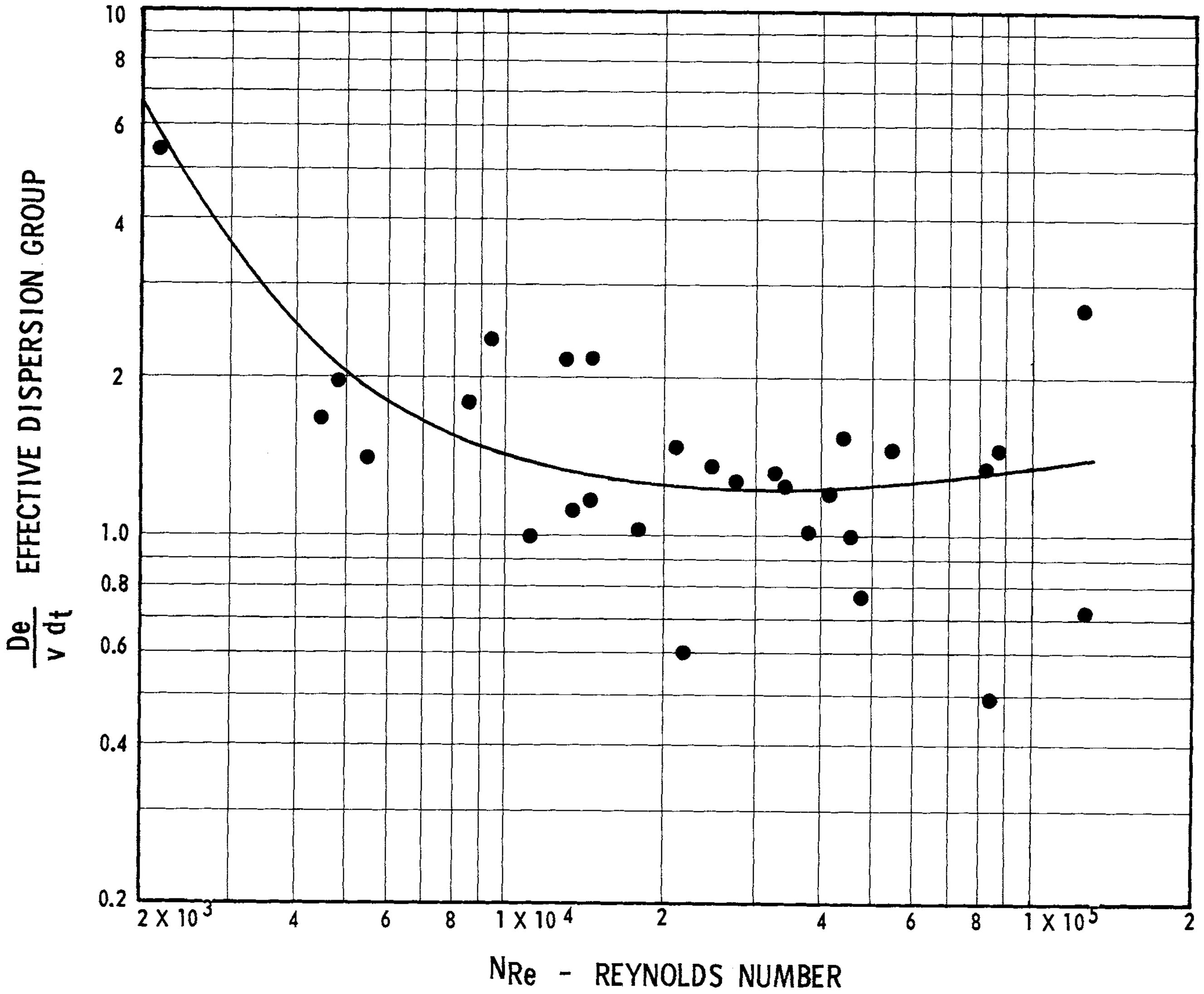

Fig. 1. Combined dispersion model fitted to Carter and Bir's data.

Substituting Equation (10) into (9) and multiplying both sides with L/d_t, we obtain

$$\frac{De}{v\,d_t} = \frac{Dp}{v\,d_t}\left(1-\frac{L_{\text{beq}}}{L}\right) + m^2\frac{D_p}{v\,d_t}\left(\frac{L_{\text{beq}}}{L}\right) \qquad (11)$$

Equation (11) can be used to determine an effective dispersion group provided the proportionality constant m is given.

RESULTS

It was found that by letting $m = 20 \ln (N_{Re}/2{,}500)^2$ and $L_{\text{beq}}/L = 0.07$, a reasonable fit was possible for Carter and Bir's data as shown in Figure 1. It was necessary to use m as a function of Reynolds numbers to produce the minimum in the dispersion group curves. The dispersion coefficients for the straight pipe were obtained from the center line of Levenspiel's curves (3).

DISCUSSION

The ability to obtain an effective dispersion coefficient that gives similar trends with Reynolds number as the experimental data is not surprising considering the flexibility available in choosing the equivalent length and the function m. However, there are concepts in the approach that are significant. First is the flexibility of a mixed dispersion model. The second is that of taking into account the mixing characteristics of pipe or vessel sections independently to predict the overall dispersion effect. The third is that if the individual mixing effects can be related to the extent of reaction, even if only in an empirical manner, a logical sequence is available to design chemical reactors taking into account nonideal flow conditions. For each section of a reactor a mixing effect would be predicted and related to a conversion for that particular section.

ACKNOWLEDGMENT

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NOTATION

D_b = axial dispersion coefficient for bend section
D_p = axial dispersion coefficient for straight pipe
D_e = effective axial dispersion coefficient for entire system
d_t = pipe diameter
L_{beq} = equivalent length of bend section

L_p = length of straight pipe section
L = total length
N_{Re} = Reynolds number
m = proportionality constant
v = mean fluid velocity
μ_p = p^{th} moment about origin (dimensionless)
σ^2 = variance (dimensionless)
Δ = difference between outlet and inlet moments

LITERATURE CITED

1. Bischoff, K. B., *A.I.Ch.E. J.*, **10**, 584 (1964).
2. Carter, D., and W. G. Bir, *Chem. Eng. Progr.*, **58**, 40 (1962).
3. Levenspiel, O., "Chemical Reaction Engineering," Wiley, New York (1962).
4. Levenspiel, O., and K. B. Bischoff, *Advanc. Chem. Eng.*, **4** (1963).

Note on the Use of Z_c as a Third Parameter with the Corresponding States Principle

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In a recent article by Reid and Leland (7), a brief comment about dimensional analysis was inserted on page 231 of the article with the statement that in a system described completely by the dimensional quantities P_c, V_c, T_c, R, P, V, T, the reduced equation of state relates the compressibility factor Z to only two independent dimensionless groups, implying that Z_c is not a variable. This statement is not correct and needs further explanation.

THE USE OF Z_c AS A THIRD PARAMETER

In empirical equations of state of the form

$$Z = f(P_R, T_R, Z_c, a_o, b_o, \ldots) \tag{1}$$

where a_o, b_o, ... are dimensionless constants obtained by fitting PVT data which do not include the critical region, extrapolation of the equation to the critical will usually determine a constant Z_c, because the setting of $Z = Z_c$, $P_R = 1$, $T_R = 1$ in Equation (1) produces

$$Z_c = f(1, 1, Z_c, a_o, b_o, \ldots) \tag{2}$$

which can be solved to give one or more constant roots for Z_c. The subscripts *o* indicate that these are universal constants applicable to all substances. However, if the critical region is included in the evaluation, the constants a_o, b_o, ... may be defined so that the values 1, 1, a_o, b_o, ... all cancel at the critical. The right side of Equation (2) then becomes only Z_c, so that the equation becomes the identity $Z_c = Z_c$ at the critical point. A method of doing this is to make three of the terms a_o, b_o, ... in Equation (1) not constants but variable universal functions of Z_c. These three terms are then defined by simultaneous solution of the equation of state with the required zero values of $(\partial P/\partial V)_T$ and $(\partial^2 P/\partial V^2)_T$ at the critical. This will define each as a function of Z_c. Substitution back into Equation (1) of all parameters defined in this way eliminates them from the equation by making them functions of Z_c. In this manner Equation (2) at the critical becomes

$$Z_c \equiv f[a_o(Z_c), b_o(Z_c), c_o(Z_c), \ldots d_o, e_o, \ldots] = Z_c \tag{3}$$

The functions $a_o(Z_c)$, $b_o(Z_c)$, $c_o(Z_c)$ will include the remaining constants d_o, e_o, ... in such a manner that they cancel at the critical and leave only Z_c on the right side of Equation (3). The equation thus becomes the identity $Z_c = Z_c$ (8).

The remaining universal constants d_o, e_o, ... can be present in any number to fit the compressibility at specific points away from the critical for various fluids. However, interpolations or extrapolations to other fluids not used to evaluate d_o, e_o, ... are determined in this case by a third parameter evaluated from the behavior of all fluids at their critical conditions. This interpolation or extrapolation to predict properties of other fluids is then assumed to be described at all conditions by the same third parameter which gives the correct interpolation at the critical. If a reduced equation with only three parameters could represent dissimilar fluids both at the critical and at low densities, this assumption would unquestionably be valid. Unfortunately, however, this is not the case. Any arbitrarily defined third parameter obtained at low densities and adjusted to fit virial coefficient data could be replaced by a function of Z_c if there is a smooth single-valued correlation of this parameter with Z_c. However, when Z_c is plotted against any third parameter which predicts low density PVT data, one obtains a scattering of points rather than a smooth curve. The higher members of the normal paraffin hydrocarbon series usually give the smoothest correlation. Hydrocarbons with other structures and other nonpolar molecules are usually scattered widely, so that two molecules with significant structural dissimilarities may have very nearly the same Z_c. Plots of this type are shown by Lydersen, Greenkorn, and Hougen (5) and by Hirschfelder et al (2).

The significance of this is that if one assumes the existence of a function

$$Z = f(T_R, P_R, Z_c) \tag{4}$$

to allow interpolation in a table of experimental values of these reduced properties, one will obtain excellent results near the critical, but interpolations made away from the critical become more and more scattered as the density decreases. This increase in scatter at low densities has been pointed out by Hougen, Watson, and Ragatz (3). The obvious conclusion is that more than three parameters are needed to account for deviations from the simple corresponding states principle over extensive density ranges.