COMMUNICATIONS TO THE EDITOR

Axial Dispersion and Void-cell Mixing Efficiency in Fluid Flow in Fixed Beds

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A most vital interest has recently been manifested in the subject of axial dispersion of fluids flowing through fixed beds. The contribution of Aris and Amundson in a recent issue of this Journal (*1*) demonstrates for an impulse input of tracer what Kramers and Alberda (*6*) showed for a sinusoidal input, namely that such a bed may be profitably viewed as a series of perfect mixers. Aris and Amundson further showed by a comparison of mixing and turbulent diffusion distribution functions that the limiting value of the Peclet number $D_p v/E$ should be about 2 in the range of fully developed turbulence in a packed bed. McHenry and Wilhelm (*7*) have demonstrated this point theoretically and, for gas systems, experimentally.

It is the purpose of this communication to supplement the aforementioned derivations by a consideration of axial dispersion in terms of a void-cell mixing-efficiency model (*2*).

THEORY

Axial dispersion of a fluid flowing through a vessel, pipe, or packed bed is conveniently defined for the moment as that phenomenon which results in a distribution of residence times for a differential element of fluid entering the apparatus. Thus, for a vessel of volume V, carrying a fluid entering at a volumetric flow rate F, the nominal holding or residence time is $V/F = \theta$. All species entering the vessel have a residence time equal to θ only if there exists a complete absence of forward and/or backward dispersion, termed *axial mixing.*

Unpacked Vessels

Consider the turbulent flow of a fluid in a pipe. If all entering masses of fluid are in residence for a time $\theta = V/F$, there is then no axial dispersion and this condition is achieved only at very high values of the Reynolds number. On the other hand consider the situation encountered in a well-stirred vessel where "perfect mixing" prevails. Clearly a wide distribution of residence times results in this case.

Defining an axial dispersion coefficient E by the differential equation

$$E \frac{\partial^2 C}{\partial X^2} - v \frac{\partial C}{\partial X} = \frac{\partial C}{\partial t}$$

one encounters the two extremes:

Piston flow $E = 0$

Perfect mixing $E \rightarrow \infty$

Consider a vessel of nominal holding time θ. If under conditions of steady state flow, a pulse of tracer material is instantaneously injected into the vessel, then the effluent concentration C as a function of time is

$$C = \frac{Q}{V} e^{-t/\theta} \qquad (1)$$

Figure 1 shows the concentration-time profile for the cases of (*a*) perfect mixing and (*b*) piston flow for an impulse input.

Packed Beds

What has been said above concerning the limits of axial dispersion in unpacked conduits can, with some qualifications, be said of packed columns. Clearly the case approaching perfect mixing ($E \rightarrow \infty$) is encountered in fluidized beds, as has been demonstrated by tracer studies (*5*).

Ergun (*4*) provided substantial evidence for the existence of near-perfect mixing in fixed-bed studies. Certainly, shallow fixed beds of large diameter exhibited perfect mixer characteristics.

The other extreme, that of piston flow in any packed bed ($E = 0$), is virtually nonexistent. This may be shown simply; as any packed bed must consist of a series of randomly arrayed void cells, it is fruitful to consider the behavior of a pulse input imposed upon a series of these bed cells, each of holding time θ_n. In this case the concentration-time behavior for the effluent of the nth perfect-mixing cell is given by

$$C = \frac{G}{\theta_n{}^n} \frac{t^{n-1} e^{-t/\theta}}{(n-1)} \qquad (2)$$

For several beds of the same total retention time T, the cell holding time is obviously $\theta_n = T/n$. Equation (2) has been solved for three equal total-volume beds composed of two, four, and twelve perfect mixers. The resulting dispersions are plotted in Figure 2. It is apparent that the minimum dispersion occurs when n is a maximum. The limit is the case of n approaching infinity. Since any real bed consists of a finite number of cells, it is clear that even in the limiting case of perfect mixing in each void cell there exists, nevertheless, a finite axial dispersion. Hence, for a bed of many

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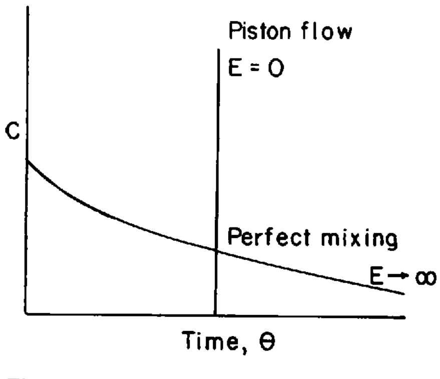

Fig. 1. Pulse dispersion for piston and perfect-mixer flow.

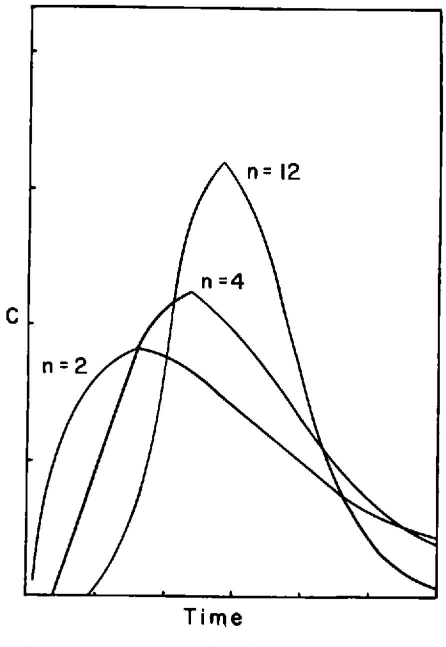

Fig. 2. Pulse dispersion in n perfect mixers. Equal total holding time.

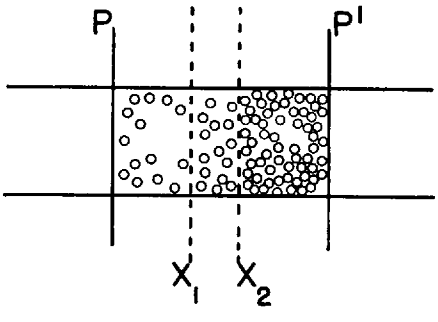

Fig. 3. Einstein's kinetic-diffusion model.

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perfect-mixing cells the axial dispersion of matter corresponds to a finite value of E.

Now consider the effects of imperfect mixing in the bed cells. Mixing efficiency is a function of turbulence and retention time for a given fluid. It follows that fluid velocity and cell size control mixing efficiency. Cell size is a function of particle diameter D_p. Thus, it may be assumed that

$$E = kD_pv \tag{3}$$

The ratio $D_pv/E = 1/k$ is defined as the Peclet number Pe.

For a given velocity a mixing time θ_p is required for perfect mixing; the time is provided by the cell dimension (a function of D_p) and the number of such cells. Imperfect mixing may therefore be characterized as the situation where the cell retention time θ_n is less than the required perfect-mixing time θ_p. Thus more than one cell is required to achieve the perfect mixing time. For a bed of n_p void cells, the effect of imperfect mixing is to endow the bed with the dispersion characteristics of a bed of n mixers. Since $n < n_p$, a greater dispersion and therefore larger E result.

Imperfect mixing may be also viewed profitably as the result of by-passing or short circuiting and dead-space retention. This simply states that of x particles entering a void cell, a fraction passes through the cell in a time much shorter than the holding time θ_n, while another fraction is retained for a period much greater than this holding time. Obviously a distribution of retention times results which is characterized by a dispersion coefficient E. The similarity of this process to molecular diffusion offers an opportunity for a more quantitative treatment.

Fick's first law of diffusion states that the rate of species transport via diffusion is proportional to the concentration gradient; that is

$$\text{rate} = -D_m \frac{dC}{dX} \tag{4}$$

where D_m is the proportionality constant, or diffusion coefficient. Consider a field of particles and a zone $(X_2 - X_1)$ bound by lines P and P' as shown in Figure 3. The transport of U molecules from left to right may be expressed, per unit area, as

$$U_a = \tfrac{1}{2}C_a(X_2 - X_1) \tag{5}$$

since it is argued that probability dictates an equal chance of molecules going in either direction.

The transport from right to left is by similar reasoning

$$U_b = \tfrac{1}{2}C_b(X_2 - X_1) \tag{6}$$

The net diffusion is then

$$U_b - U_a = \tfrac{1}{2}(X_2 - X_1)(C_b - C_a) \tag{7}$$

Now if $X_2 - X_1$ is small, Fick's first law may be written as

$$\text{rate} = D_m \frac{(C_b - C_a)}{(X_2 - X_1)} \tag{8}$$

The rate of net transport in a time interval θ_D is

$$(\text{rate})\theta_D = D_m \frac{(C_b - C_a)}{(X_2 - X_1)} (\theta_D) \tag{9}$$

Since rate $\theta_D = U_b - U_a$, then

$$D_m \frac{(C_b - C_a)}{(X_2 - X_1)} \theta_D = \tfrac{1}{2}(X_2 - X_1)(C_b - C_a) \tag{10}$$

which results in

$$D_m = \frac{(X_2 - X_1)^2}{2\theta_D} \tag{11}$$

The diffusion time constant is thus

$$\theta_D = \frac{(X_2 - X_1)^2}{2D_m}, \tag{12}$$

the well-known Einstein relationship.

Relations for a Real Bed

If a packed bed of length L, containing n mixing units, is visualized, then the height of one mixer is L/n. Since the mixing coefficient E is a measure of up- and downstream dispersion or diffusion, the time constant for axial mixing may be written

$$\theta_a = \frac{(L/n)^2}{2E} \tag{13}$$

Fluid retention or holding time per mixing length for a bed velocity v is

$$\theta_n = \frac{L/n}{v} \tag{14}$$

As a perfect mixer is one in which retention and mixing times are equal, then

$$\frac{L/n}{v} = \frac{(L/n)^2}{2E} \tag{15}$$

and the number of mixers in terms of L, v, and E is

$$n = \frac{Lv}{2E} \tag{16}$$

As $E \to \infty$ for $n = 1$, then for a small number of mixers (*6*), Equation (16) is best written

$$n - 1 = \frac{Lv}{2E} \tag{16a}$$

From Equation (16) it follows that the height of a mixing unit is given by

$$\text{H.M.U.} = 2E/v \tag{17}$$

Ideal Bed Model

Consider now a bed in which each cell is a perfect mixer formed by particles of diameter D_p. The length of each perfect mixing cell will be some fraction γ of particle diameter D_p (*1*). This fraction γ will be about unity or less, depending on the packing arrangements; therefore, the number of perfect mixers is

$$n_p = L/(\gamma\ D_p) \tag{18}$$

For any bed, one may define a mixing efficiency as the ratio of actual mixers n to the limiting number in the perfect-mixing–cell case n_p:

Mixing efficiency $e = n/n_p$ or

$$e = (Lv/2E)/(L/\gamma D_p) = D_p v/2E \tag{19}$$

Since $D_p v/E = Pe$, then

$$e = (\gamma/2)Pe \tag{20}$$

As γ is a constant for a fixed bed, then Equation (20) expresses the quantitative relationship between the Peclet number for axial dispersion and void-cell mixing efficiency. Further, the limiting value of the Peclet number is easily predicted from the foregoing argument, for as the void cells approach the perfect-mixer ideal, $e \longrightarrow 1$ and

$$Pe = 2/\gamma \tag{21}$$

Since γ is approximately 1, then the limiting value of the Peclet number is about 2. Equation (21) can be rewritten

$$Pe = 2/(\gamma/e) \tag{22}$$

if

$$\gamma/e = l \tag{23}$$

Then l is simply a measure of mixing length for any bed.

$$l = 2/Pe = 2E/D_p v \tag{24}$$

i.e., l is the number of particle diameters equivalent to one mixing unit.

Since by Equation (17) H.M.U. $= 2E/v$ then

$$l = \text{H.M.U.}/D_p \tag{25}$$

Thus by utilization of Einstein's simple diffusion model in terms of mixing inefficiency in a void cell, it is shown how the Peclet number is directly related to void-cell mixing efficiency in a packed bed; further, the limiting value of the Peclet number is derived in a manner which is both simple and logical.

In addition, insofar as the friction factor for packed beds reflects to some degree cell turbulence in terms of expansion and contraction losses, one may predict a marked decrease in the height of a mixing unit as the character of fluid flow approaches the regime of incipient and developed turbulence in a packed bed. It follows that significantly high values of H.M.U. will be encountered in the low flow regions usually employed in many fixed-bed processes such as ion exchange. Results of axial dispersion studies (*2*) soon to be published (*3*) confirm these comments.

NOTATION

C = concentration of tracer
D_p = particle diameter, length
D_m = molecular diffusivity, length²/time
e = cell mixing efficiency
E = axial dispersion coefficient, length²/time
F = volumetric flow rate, volume/time
G = constant
H.M.U. = height of a mixing unit, length
k = proportionality constant, Equation (3)
l = number of particle diameters per mixing length
L = bed length
n = number of mixers, $L_v/2E$
n_p = number of perfect mixers, $L/\gamma D_p$
Pe = Peclet number, $D_p v/E$
Q = quantity of injected tracer
t = time
T = total residence time
U = number of particles transported in a diffusion field
v = average fluid velocity in packed bed, length/time
V = vessel volume
X = distance parameter in Einstein model
γ = fraction of a particle diameter equal to a perfect-mixer length
θ = holding time
θ_n = cell holding time
θ_p = perfect mixing time

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because of the uncertainties in the approximations involved; the very good agreement with experimental results is probably fortuitous. However, even if somewhat different approximations had been used, the order of magnitude would still have been correct.

An interesting consequence of the mixing-length model is that it provides a qualitative prediction of the effect of void fraction on the axial Peclet group. As the void fraction rises, the bed becomes more loosely packed. The mixing-length model suggests that this loosening is accompanied by a small decrease in the velocity gradient and a slight increase in radial scale l_r. To a first approximation these effects will tend to cancel one another. However, the axial scale l_z, which is a measure of the by-passing length, would be expected to increase considerably. As a result the model predicts that an increase in void fraction produces a larger axial eddy diffusivity or a smaller Peclet group. Current experimental work (*1*) at Berkeley confirms this result.

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