# A Crossflow Model of Dispersion in Packed Bed Reactors

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A three-parameter model of axial and radial dispersion in a packed tubular reactor is proposed as an alternative to the Fickian dispersion model. Though it is formulated in terms of differential equations, it requires no exit boundary condition, so it is mathematically more convenient than the Fickian model. Examples of its application to chemical reactors are given.

## SCOPE

Dispersion in packed beds can be modelled as a Fickian diffusion process or as flow through an interconnected network of stirred tanks. The former type of model has the disadvantage that it requires a boundary condition at the exit from the bed. This is both physically and mathematically troublesome. Also, upstream diffusion from the point of injection of a tracer pulse is predicted, whereas observations show virtually none. Models of the second type, on the other hand, need only inlet boundary conditions and do not predict upstream dispersion. They are, however, formulated in terms of recurrence relations, which are often less convenient mathematically than differential equations.

Investigated here is a dispersion model which takes the form of differential equations, but requires only inlet boundary conditions and predicts no upstream dispersion. It also predicts a finite downstream propagation velocity for an injected tracer pulse. The model has three dimensionless parameters which characterize axial and radial dispersion, and methods of estimating these parameters are discussed. Finally, the equations are applied to two examples of chemical reaction in a packed tubular reactor, and results are compared with the predictions of the plug flow model and the Fickian dispersion model.

## CONCLUSIONS AND SIGNIFICANCE

The crossflow dispersion model developed here has been shown to respond to an injected tracer pulse in a manner which quickly approaches the response of the Fickian dispersion model, except that there is no upstream spreading, and the downstream propagation velocity is bounded. Analysis of the performance of a tubular chemical reactor with sequential first-order reactions gives results which do not differ greatly from those predicted by a Fickian dispersion model with suitably matched Peclet number.

Thus the value of the model lies not in predictions of new physical behavior, but in the mathematical simplicity of the equations it yields for chemical reactors. These require no exit boundary condition and, in isothermal cases, they have explicit solutions which can quickly be obtained, even for cases where the Fickian dispersion model leads to impossibly unwieldy algebraic manipulations.

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Dispersion in a packed bed is most commonly modelled by introducing the second derivatives of concentration (with respect to spatial co-ordinates) into the material balance equations, in the form of terms the same as those which describe Fickian diffusion. In dimensionless terms, dispersion can then be characterized by axial and radial Peclet numbers, corresponding to dispersion parallel and normal to the direction of convective flow, respectively. While this is a sound description of dispersion by a true molecular diffusion process, it has a number of disadvantages as a description of the flow patterns which are the principal causes of dispersion in packed beds. For example, it predicts spreading of an injected pulse of tracer with a formally infinite velocity in all directions from the point of injection. In particular, this implies that the pulse will spread upstream from its injection point. In practice, however, upstream spreading is not observed (except possibly a very small amount due to molecular diffusion), and the tracer front propagates even downstream with a bounded velocity.

Mathematically, the presence in the equation of a second derivative with respect to axial distance means that a boundary condition must be specified at the exit from the bed, to determine a solution uniquely. This is in addition to the familiar material balance condition at the inlet. The exit condition is usually taken to require that the axial derivative of concentration should vanish, but this condition has been the subject of a good deal of discussion, and it has no clear counterpart in the physical situation. When modelling chemical reactions in a packed bed, the presence of the second spatial derivatives and the associated two-point boundary conditions leads to cumbersome algebraic manipulations when explict solutions are possible, and to more extensive computations to obtain a numerical solution.

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These disadvantages have led to the introduction of alternative models which do not require exit boundary conditions, for example, mixing-cell models of the type developed by Deans and Lapidus (1960a, b). In these, the bed is modelled as an interconnected set of perfectly mixed regions representing the interstices between packing elements. This model is described by recurrence relations, rather than differential equations. Further, on passing to the limit as the number of mixing cells increases and the size of each cell decreases, these difference equations reduce to the differential equations of a plug flow reactor. So, a dispersion model cannot be obtained by this limiting process.

It is possible to retain axial dispersion on passing to the limit of a large number of small mixing cells, but only by introducing suitable recycle flows between successive cells. Then the limiting differential equations obtained are those of the Fickian dispersion model, so the mathematical advantage of the mixing cell model is lost.

The mixing cell model was later extended by Deans (1963), who introduced the idea that part of the fluid in each cell might be regarded as stagnant, with the regions occupied by stagnant and flowing fluid linked by an exchange of material. The limit of Deans' model as the number of mixing cells becomes very large is the same as the one-dimensional special case of the model which will be proposed in this article. Deans' model was later re-analyzed by Levich et al. (1967), using a stochastic argument.

Mathematically, it is convenient to have a model which describes the behavior of the bed in terms of differential equations and it is desirable that the model should also have the following properties:

(a) its differential equations should require boundary conditions only at the reactor inlet, so that their solution poses an initial value problem,

(b) it should predict no spreading of an injected tracer pulse upstream from the injection point, and

(c) it should predict a finite downstream propagation velocity for a front of injected tracer.

A model with these properties will be described here. Physically, it is based on an idealization of the flow pattern in the bed by classifying the whole void region into "stagnant" and "flowing" parts. The stagnant parts correspond to the wakes of packing elements, and dispersion is introduced by assuming that there is exchange of fluid between the stagnant and flowing regions throughout the bed. This idea has previously been used to explain dispersion effects in the liquid phase of a trickle bed (Hoogendorn and Lips (1965), Hochman and Effron (1969), Bennet and Goodridge (1970)), but physically it seems equally reasonable to use it in describing single phase flow in a packed bed. The term "crossflow model" was used in the above publications to describe this picture of dispersion, and the same name will be used here to describe our model of dispersion in single phase flow.

## FORMULATION OF A MODEL

It will be assumed that fluid flows through the bed in the direction of the $z$-axis, the volume flow rate per unit total cross-sectional area being denoted by $\bar{u}$, supposed independent of $x$ and $y$. Though the detailed flow pattern in the bed is complicated, we idealize it by classifying the interstitial region into "stagnant" and "flowing" parts. The volumes occupied by these regions, respectively, per unit total bed volume, will be denoted by $\epsilon_b$ and $\epsilon_a$. Then clearly $\epsilon_a + \epsilon_b = \epsilon$, where $\epsilon$ is the void fraction of the bed.

The stagnant regions represent "wakes" of the solid particles in the bed, though the particles are so close together in a packed bed that it is not possible to identify each wake unambiguously with a corresponding particle. The fluid is by no means at rest everywhere in the wakes. On the contrary, they may contain quite vigorous circulation patterns. Still, it is assumed that the local mean value of the fluid velocity in the 'stagnant' regions vanishes, where averaging is over a domain containing a representative selection of these regions.

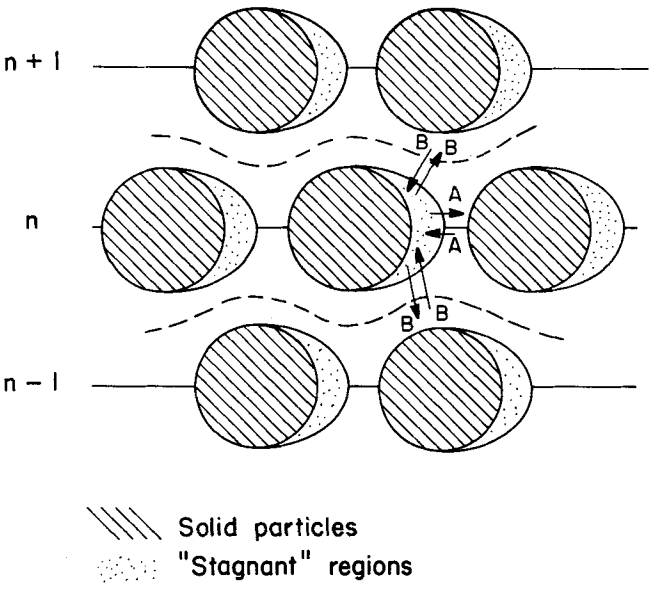


**Figure 1. Schematic of bed showing stagnant and flowing regions. ⇄A indicates exchange between stagnant and flowing regions in the same layer. ⇄B indicates exchange between stagnant and flowing regions in adjacent layers.**

The local average value of the fluid velocity in the 'flowing' region will be denoted by $\mathbf{v}$. It is directed along the $z$-axis and has magnitude $v$, where $\epsilon_a v = \bar{u}$. We further assume that flowing and stagnant regions are not mutually isolated, but that fluid is exchanged between them at a volumetric rate $f$ per unit bed volume. Physically, this corresponds to wake shedding and re-entrainment.

We shall consider the transport of a solute present in small concentration in the fluid, denoting by $c$ and $\bar{c}$ its local average concentrations in the flowing and stagnant regions, respectively. Initially it will be assumed that $c$ and $\bar{c}$ are independent of the co-ordinate $x$, so the problem can be analyzed in two space dimensions. An appropiate generalization to three dimensions is then simple.

For a regular packing, the bed can be divided into geometrically similar layers, which differ only by a translation parallel to the $y$-axis. Denote the smallest thickness for such layers by $\lambda$. The value of $\lambda$ depends on the particular packing arrangement and the orientation of the $y$ and $z$ axes, but it is of the order of the particle diameter. In the case of a random packing, the geometric similarity of different layers must be interpreted statistically.

Layers will be numbered in order of increasing $y$, and the symbols $c_n$ and $\bar{c}_n$ will be used to denote the values of $c$ and $\bar{c}$ at the center plane of the $n^{\text{th}}$ layer. These concentrations will then be associated with all the flowing and stagnant fluid, respectively, in this layer. These ideas are illustrated schematically by Figure 1.

Now consider material balances for solute in the flowing and stagnant fluid in an element of the $n^{\text{th}}$ layer of thickness $\delta z$, measured parallel to $z$-axis, and unit width in the direction of the $x$-axis. $\delta z$ is large enought that this element contains a representative sample of the layer. Then solute is transported to and from the flowing fluid in the element by the following processes:

(a) Convective transport associated with the flowing stream.

(b) Exchange of fluid with stagnant regions in the same layer.

(c) Exchange of fluid equally with stagnant regions in each adjacent layer.

(d) Generation or consumption by chemical reaction.

If we suppose a fraction $\alpha$ of the stagnant fluid entering the flowing stream comes from stagnant regions in the same layer, while a fraction $(1-\alpha)$ comes from stagnant regions in adjacent layers, the material balance equation is

$$\epsilon_a \lambda \delta z \frac{\partial c_n}{\partial t} = \epsilon_a \lambda v c_n(z) - \epsilon_a \lambda v c_n(z+\delta z)$$

$$+ \lambda\delta z\alpha f\bar{c}_n(z) + \lambda\delta z\frac{1}{2}(1-\alpha)f[\bar{c}_{n+1}(z) + \bar{c}_{n-1}(z)]$$
$$- \lambda\delta z f c_n(z) + \epsilon_a\lambda\delta z R[c_n(z)] \quad (1)$$

where $R$ denotes the rate of generation of solute per unit fluid volume by chemical reaction. Passing to the limit $\delta z \to 0$, Equation (1) becomes

$$\frac{\partial c_n}{\partial t} + v\frac{\partial c_n}{\partial z} + \frac{f}{\epsilon_a}\{c_n - \alpha\bar{c}_n - \frac{1}{2}(1-\alpha)[\bar{c}_{n+1} + \bar{c}_{n-1}]\} = R(c_n) \quad (2)$$

For stagnant fluid in the element, solute is transported by (a) exchange of fluid with flowing regions in the same layer, (b) exchange of fluid equally with flowing regions in each adjacent layer, and (c) generation or consumption in chemical reactions. Then if a fraction $\beta$ of the flowing fluid entering the stagnant region comes from flowing regions in the same layer and a fraction $(1-\beta)$ from flowing regions in adjacent layers, the material balance equation corresponding to (2) above is

$$\frac{\partial \bar{c}_n}{\partial t} + \frac{f}{\epsilon_b}\{\bar{c}_n - \beta c_n - \frac{1}{2}(1-\beta)[c_{n+1} + c_{n-1}]\} = R(\bar{c}_n) \quad (3)$$

Now, if $y$ is the co-ordinate of the center plane of the $n^{\text{th}}$ layer, $y + \lambda$ and $y - \lambda$ are the co-ordinates of the center planes of the adjacent layers, and we can write

$$c_n(z) = c(y,z);\ c_{n+1}(z) = c(y+\lambda,z);\ c_{n-1}(z) = c(y-\lambda,z) \quad (4)$$

and similarly for $\bar{c}$. Furthermore, since $c$ and $\bar{c}$ represent local average concentrations over domains containing representative samples of flowing and stagnant regions, the spatial variation of these variables will be smooth and quite small over distances of the order of $\lambda$. Thus it is reasonable to expand $c(y \pm \lambda, z)$ in truncated Taylor series about the point $(y,z)$, giving

$$c_{n+1}(z) = c(y+\lambda,z) = c(y,z) + \lambda\frac{\partial c}{\partial y} + \frac{1}{2}\lambda^2\frac{\partial^2 c}{\partial y^2}$$

$$c_{n-1}(z) = c(y-\lambda,z) = c(y,z) - \lambda\frac{\partial c}{\partial y} + \frac{1}{2}\lambda^2\frac{\partial^2 c}{\partial y^2}$$

where the derivatives $\partial c/\partial y$ and $\partial^2 c/\partial y^2$ are evaluated at $(y,z)$. Thus,

$$\frac{1}{2}[c_{n+1}(z) + c_{n-1}(z)] = c(y,z) + \frac{1}{2}\lambda^2\frac{\partial^2 c}{\partial y^2}(y,z) \quad (5)$$

and, similarly

$$\frac{1}{2}[\bar{c}_{n+1}(z) + \bar{c}_{n-1}(z)] = \bar{c}(y,z) + \frac{1}{2}\lambda^2\frac{\partial^2 \bar{c}}{\partial y^2}(y,z) \quad (6)$$

Using (4), (5) and (6), Equations (2) and (3) can then be written

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial z} + \frac{f}{\epsilon_a}(c-\bar{c}) - (1-\alpha)\frac{f\lambda^2}{2\epsilon_a}\frac{\partial^2 \bar{c}}{\partial y^2} = R(c) \quad (7)$$

and

$$\frac{\partial \bar{c}}{\partial t} + \frac{f}{\epsilon_b}(\bar{c}-c) - (1-\beta)\frac{f\lambda^2}{2\epsilon_b}\frac{\partial^2 c}{\partial y^2} = R(\bar{c}) \quad (8)$$

These are basic equations of the model, but it is useful to consider special cases. For example, if $\alpha = \beta = 1$ there is no dispersion perpendicular to the direction of flow, as might be expected since transfer between stagnant and flowing regions then occurs without lateral displacement. $\alpha = \beta = 0$, on the other hand, gives a maximum amount of lateral dispersion for given values of the remaining parameters. Particularly simple equations, which still include lateral dispersion, are obtained by taking $\alpha = 0$, $\beta = 1$, or $\alpha = 1$, $\beta = 0$. Then a term representing dispersion in the $y$-direction appears in only one of the equations. In particular, the latter choice gives the following equations

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial z} + \frac{f}{\epsilon_b}(c-\bar{c}) = R(c) \quad (9)$$

and

$$\frac{\partial \bar{c}}{\partial t} + \frac{f}{\epsilon_b}(\bar{c}-c) - \frac{f\lambda^2}{2\epsilon_b}\frac{\partial^2 c}{\partial y^2} = R(\bar{c}) \quad (10)$$

which will be used in the rest of this paper.

The advantage of making a particular choice of values for $\alpha$ and $\beta$ is that it reduces the number of free parameters in the model. Thus, since $v = \bar{u}/\epsilon_a$ and $\epsilon_a + \epsilon_b = \epsilon$, Equations (9) and (10) contain three parameters $f$, $\epsilon_b$ and $\lambda$, which characterize the dispersion.

For a three dimensional system with $z$-axis aligned with the direction of flow, it is necessary only to replace Equation (10) by

$$\frac{\partial \bar{c}}{\partial t} + \frac{f}{\epsilon_b}(\bar{c}-c) - \frac{f\lambda^2}{2\epsilon_b}\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) = R(\bar{c}) \quad (10')$$

and no new parameters appear.

Equations (9) and (10) must be compared with the familiar equation for the Fickian model of dispersion, namely

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial z} - D_z\frac{\partial^2 c}{\partial z^2} - D_t\frac{\partial^2 c}{\partial y^2} = R(c) \quad (11)$$

where $u$ is the interstitial average fluid velocity, defined by $u = \bar{u}/\epsilon$, and $D_z$ and $D_t$ are axial and transverse dispersion coefficients, respectively. This contains only two parameters, $D_z$ and $D_t$, in contrast to the three parameters of the present model. But it also contains the second spatial derivative in the $z$-direction, which means that, to determine a solution, an exit boundary condition must be postulated, in addition to the upstream conditions.

The dimensionless form of Equation (11) is well known. Introducing dimensionless co-ordinates and dimensionless time, defined by

$$\xi = x/d,\ \eta = y/d,\ \zeta = z/d,\ \tau = ut/d \quad (12)$$

where $d$ is a suitably defined length characteristic of the packing material, the equation can be written

$$\frac{\partial \gamma}{\partial \tau} + \frac{\partial \gamma}{\partial \zeta} - \frac{1}{Pe_z}\frac{\partial^2 \gamma}{\partial \zeta^2} - \frac{1}{Pe_t}\frac{\partial^2 \gamma}{\partial \eta^2} = \mathcal{R}(\gamma) \quad (13)$$

where $\gamma$ is a dimensionless concentration and $\mathcal{R}$ a dimensionless reaction rate, defined by

$$\gamma = c/c_0, \qquad \mathcal{R} = dR/uc_0 \quad (14)$$

with $c_0$ denoting a reference concentration; for example, the concentration in the entering stream. Dispersion is characterized by the axial and transverse Peclet numbers

$$Pe_z = ud/D_z, \qquad Pe_t = ud/D_t \quad (15)$$

The corresponding dimensionless form of Equations (9) and (10) is

$$(1-S)\frac{\partial \gamma}{\partial \tau} + \frac{\partial \gamma}{\partial \zeta} + F(\gamma - \bar{\gamma}) = (1-S)\mathcal{R}(\gamma) \quad (16)$$

$$S\frac{\partial \bar{\gamma}}{\partial \tau} + F(\bar{\gamma} - \gamma) - \frac{1}{2}FL\frac{\partial^2 \bar{\gamma}}{\partial \eta^2} = S\mathcal{R}(\bar{\gamma}) \quad (17)$$

These equations contain three dimensionless groups, namely

$$S = \epsilon_b/\epsilon,\ F = \frac{df}{\bar{u}},\ L = \left(\frac{\lambda}{d}\right)^2 \quad (18)$$

$S$ represents the volume fraction of the fluid which is regarded as "stagnant", $F$ is a dimensionless measure of the rate of exchange of fluid between the stagnant and flowing regions, per unit bed volume, and $L$ is the square of the ratio of the effective layer thickness in the bed to the characteristic dimension of the packing. Since $\epsilon_a/\epsilon = 1 - \epsilon_b/\epsilon$, this is not an independent dimensionless parameter.

For the one-dimensional case when $\gamma$ is independent of $\eta$, Equations (16) and (17) reduce to

$$(1-S)\frac{\partial \gamma}{\partial \tau} + \frac{\partial \gamma}{\partial \zeta} + F(\gamma - \bar{\gamma}) = (1-S)\mathcal{R}(\gamma) \tag{19}$$

$$S\frac{\partial \bar{\gamma}}{\partial \tau} + F(\bar{\gamma} - \gamma) = S\mathcal{R}(\bar{\gamma}) \tag{20}$$

which are a pair of hyperbolic first order partial differential equations, whose characteristic directions are $d\zeta/d\tau = 0$ and $d\zeta/d\tau = 1/(1-S) = \epsilon/\epsilon_a$. The corresponding directions in the dimensional $(z,t)$ plane are $dz/dt = 0$ and $dz/dt = v$. Thus, if a distribution of solute is confined to an interval $z_1 < z < z_2$ at $t = 0$, with $c = 0$ elsewhere, $c$ will remain zero at all times for $z < z_1$ and for $z > z_2 + vt$. Equations (19) and (20) therefore describe a process of convection and dispersion in which there is no backmixing relative to the packing, and the concentration front is propagated downstream with a finite velocity. Both these properties contrast with Fickian dispersion.

The description of dispersion provided by Equations (16) and 17) will be referred to as the crossflow model.

## RESPONSE TO AN INJECTED PULSE

Dispersion is often investigated experimentally by injecting a sharp pulse of tracer material and observing its movement and spread with the passage of time. Here, we are interested in both axial and radial spreading, and each will be considered separately.

To investigate axial spreading a pulse is injected at the inlet to the bed ($\zeta = 0$) at the time zero, and the tracer concentration is independent of $\eta$ or $\xi$. It is then possible to observe the concentration as a function of $\zeta$ at a sequence of succeeding times, or the concentration as a function of $\tau$ at a seqence of fixed locations with increasing values of $\zeta$.

Taking the latter point of view, successive moments of the tracer concentration distribution can easily be obtained from the Laplace transform of the tracer concentration with respect to time

$$\mathcal{L}(s,\zeta) = \int_0^\infty e^{-s\tau}\gamma(\tau,\zeta)\,d\tau \tag{21}$$

for then it is well-known that

$$\bar{\tau} = -\mathcal{L}'(0,\zeta),\ \bar{\tau}^2 = \mathcal{L}''(0,\zeta) \tag{22}$$

and so forth. Hence the second moment about the mean is given by

$$\sigma^2 = \bar{\tau}^2 - (\bar{\tau})^2 = \mathcal{L}''(0,\zeta) - [\mathcal{L}'(0,\zeta)]^2 \tag{23}$$

Setting $\mathcal{R} = 0$, Equations (19) and (20) above reduce to

$$\frac{\partial \gamma}{\partial \tau} + \frac{\epsilon}{\epsilon_a}\frac{\partial \gamma}{\partial \zeta} + \frac{\epsilon}{\epsilon_a}F(\gamma - \bar{\gamma}) = 0 \tag{24}$$

$$\frac{\partial \bar{\gamma}}{\partial \tau} + \frac{\epsilon}{\epsilon_b}F(\bar{\gamma} - \gamma) = 0 \tag{25}$$

and, taking the Laplace transform with respect to time, it is easily found that

$$\mathcal{L}(s,\zeta) = \exp\left[-\left\{\frac{s^2 + F(\epsilon/\epsilon_a + \epsilon/\epsilon_b)s}{(s + F\epsilon/\epsilon_b)\,\epsilon/\epsilon_a}\right\}\zeta\right] \tag{26}$$

Using Equation (22) it then follows that

$$\bar{\tau} = \zeta;\ \bar{\tau}^2 = \frac{2(\epsilon_b/\epsilon)^2\zeta}{F} + \zeta^2$$

and hence

$$\sigma^2 = \frac{2(\epsilon_b/\epsilon)^2\zeta}{F} \tag{27}$$

A corresponding analysis for the Fickian equation

$$\frac{\partial \gamma}{\partial \tau} + \frac{\partial \gamma}{\partial \zeta} - \frac{1}{Pe_z}\frac{\partial^2 \gamma}{\partial \zeta^2} = 0$$

with pulse injection at the inlet of an infinitely long bed leads to the well known result

$$\sigma^2 = \frac{2\zeta}{Pe_z} \tag{28}$$

It is therefore possible (though, of course, not necessary) to choose the parameters of the two models in such a way as to predict the same rate of axial spreading of an injected pulse, as judged by the second moment about the mean (with respect to $\tau$) of $\gamma(\tau,\zeta)$. Identifying the values of $\sigma^2$ given by (27) and (28) gives

$$Pe_z = F\left(\frac{\epsilon}{\epsilon_b}\right)^2 = \frac{F}{S^2} \tag{29}$$

An alternative view of pulse spreading is observing the spatial distribution of tracer concentration as a function of time. The dispersion can then be measured by $\sigma'^2$, the second spatial moment of this distribution about its mean. If this quantity is calculated for the present model and the Fickian model, respectively, the following results are obtained for sufficiently large $\tau$ (Hinduja 1977)

$$\sigma'^2 \approx \frac{2(\epsilon_b/\epsilon)^2\tau}{F};\ \sigma'^2 \approx \frac{2\tau}{Pe_z}\quad (\tau \to \infty) \tag{30}$$

Identifying these values leads to the same relation (29) between the parameters of the two models.

With the parameters matched by Equation (29), it is interesting to compare the complete solutions of the equations describing the two models for the case of a delta function pulse of tracer injected at $\zeta = 0$ at time $\tau = 0$. In both, a total amount $m$ of the tracer, per unit cross-sectional area, is injected at the origin $\zeta = 0$ at time $\tau = 0$. For the crossflow model, it is also necessary to prescribe how this tracer is distributed between the stagnant and flowing regions, and we shall assume that the concentration is the same for both regions at the time of injection. The proportions entering the stagnant and flowing regions are then $\epsilon_b m/\epsilon$ and $\epsilon_a m/\epsilon$, respectively.

Deans (1963) indicated the nature of the solution of Equations (24) and (25) for this case, and it has the following explicit form

$$\gamma = \frac{m}{c_0 d}\frac{F\epsilon_a}{\epsilon}e^{-2F\zeta}e^{-\frac{F\epsilon}{\epsilon_b}(\tau-\zeta)}\left\{\frac{X}{(\tau - \epsilon_a\zeta/\epsilon)}I_1(2FX) + \frac{\epsilon}{\epsilon_a}I_0(2FX) + \frac{1}{F}\delta(\tau - \epsilon_a\zeta/\epsilon)\right\} \tag{31}$$

and

$$\bar{\gamma} = \frac{m}{c_0 d}\frac{F\epsilon_a}{\epsilon_b}e^{-2F\zeta}e^{-\frac{F\epsilon}{\epsilon_b}(\tau-\zeta)}\left\{I_0(2FX) + \frac{\epsilon_b}{\epsilon_a\zeta}XI_1(2FX)\right\} + \frac{m}{c_0 d}e^{-\frac{F\epsilon}{\epsilon_b}\tau}\delta(\zeta) \tag{32}$$

where

$$X = \sqrt{\epsilon\zeta/\epsilon_b(\tau - \epsilon_a\zeta/\epsilon)} \tag{33}$$

and $I_0$ and $I_1$ are the modified Bessel functions of zeroth and first order, respectively.

For the Fickian model, on the other hand, with the same pulse injection of tracer, the corresponding solution is

$$\gamma_f = \frac{m}{c_0 d}\sqrt{\frac{Pe_z}{4\pi\tau}}e^{\frac{-Pe_z(\tau-\zeta)^2}{4\tau}} \tag{34}$$

It is interesting to compare these two solutions, with the parameters of the two models related by Equation (29), so that second moments of the tracer distribution are matched in the two cases. An analytical method which draws fluid from a region containing a representative number of packing elements would

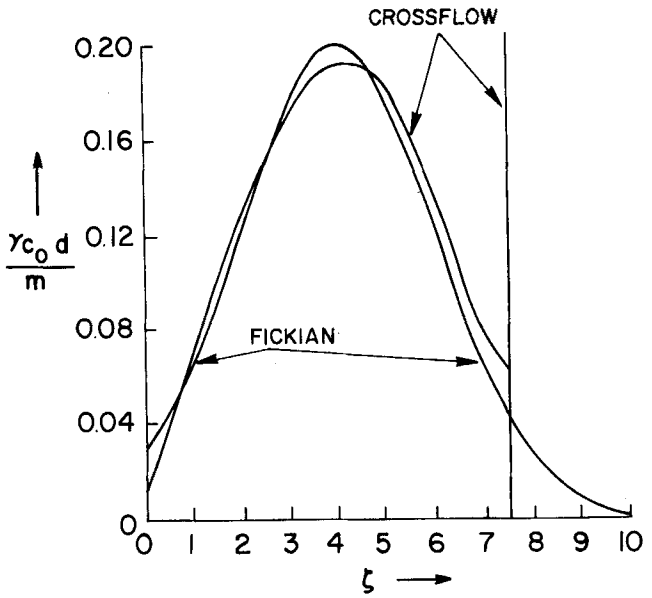


Figure 2. Pulse responses for Fickian and crossflow models. $\tau = 4$, $Pe_z = 2$, $S = 0.463$, $F = 0.429$.

measure an average of $\gamma$ and $\bar{\gamma}$, so we define

$$\gamma_m = \epsilon_a\gamma/\epsilon + \epsilon_b\bar{\gamma}/\epsilon \tag{35}$$

and compare this with $\gamma_f$, the concentration given by the Fickian result (34). In making this comparison the following parameter values were taken

$$Pe_z = 2,\ S = 0.463,\ F = 0.429$$

and these are consistent with Equation (29). Figures 2, 3 and 4 show the tracer profiles, with $\gamma_m c_0 d/m$ and $\gamma_f c_0 d/m$ plotted as functions of $\zeta$ for $\tau = 4$, 8 and 40, respectively. The delta-function spike at the leading edge of the profile for the crossflow model is indicated by a vertical line, and there is a second spike at the origin. Both these spikes become weaker, of course, as $\tau$ increases, and the continuous part of the distribution predicted by the crossflow model closely approximates that predicted by the Fickian model as $\tau$ increases. Indeed, for large $\tau$ and $|(\tau - \zeta)/\tau| << 1$ it can be shown algebraically that the two distributions coincide (Hinduja 1977). Nevertheless, the $\gamma_m$-profile remains strictly zero for $\zeta < 0$ at all times, and it has a sharp leading edge which moves at a finite velocity.

Dispersion transverse to the direction of flow may also be investigated by a pulse response method. A delta-function pulse of tracer is injected on the plane $\eta = 0$ at time zero, and its spreading in the $\eta$-direction is investigated as time increases. In this case, the solution is independent of $\zeta$, so Equations (16) and (17) reduce to

$$\frac{\partial\gamma}{\partial\tau} + \frac{\epsilon F}{\epsilon_a}(\gamma - \bar{\gamma}) = 0 \tag{36}$$

and

$$\frac{\partial\bar{\gamma}}{\partial\tau} + \frac{\epsilon F}{\epsilon_b}(\bar{\gamma} - \gamma) - \frac{1}{2}\frac{\epsilon FL}{\epsilon_b}\frac{\partial^2\gamma}{\partial\eta^2} = 0 \tag{37}$$

while the initial conditions are $\gamma(\eta, 0) = \bar{\gamma}(\eta, 0) = \delta(\eta)$. The spatial moments of the tracer profiles $\gamma$ and $\bar{\gamma}$ are defined by

$$\mu_n(\tau) = \int_{-\infty}^{\infty}\eta^n\gamma(\eta,\tau)d\eta;\ \bar{\mu}_n(\tau) = \int_{-\infty}^{\infty}\eta^n\bar{\gamma}(\eta,\tau)\,d\eta \tag{38}$$

and, multiplying each of Equations (36) and (37) by $\eta^n$ and integrating from $-\infty$ to $+\infty$, the following ordinary differential equations are obtained for the successive moments

$$\frac{d\mu_n}{d\tau} + \frac{\epsilon F}{\epsilon_a}(\mu_n - \bar{\mu}_n) = 0 \tag{39}$$

$$\frac{d\bar{\mu}_n}{d\tau} + \frac{\epsilon F}{\epsilon_b}(\bar{\mu}_n - \mu_n) - \frac{1}{2}\frac{\epsilon FL}{\epsilon_b}\,n(n-1)\mu_{n-2} = 0 \tag{40}$$

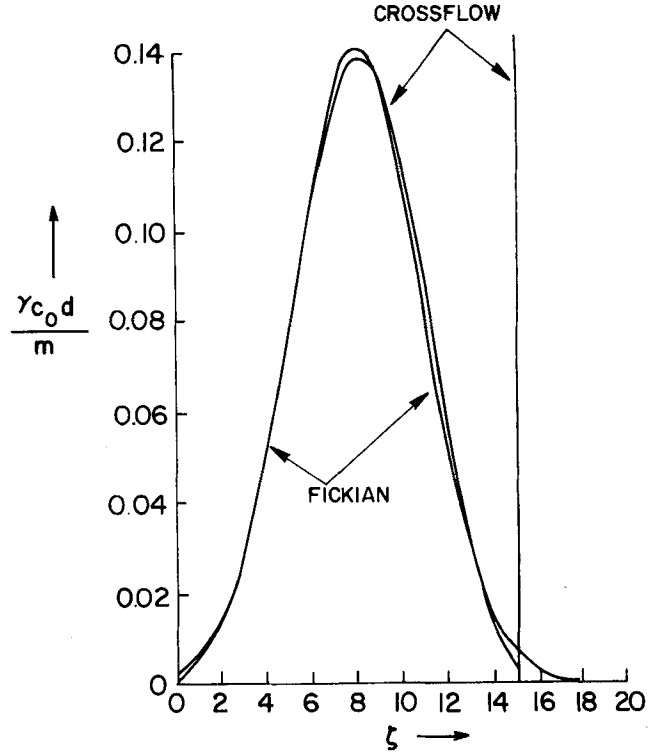


Figure 3. Pulse responses for Fickian and crossflow models. $\tau = 8$, $Pe_z = 2$, $S = 0.463$, $F = 0.429$.

These may be solved with initial conditions $\mu_0(0) = 1$; $\mu_n(0) = 0 (n > 0)$; $\bar{\mu}_0(0) = 1$; $\bar{\mu}_n(0) = 0 (n > 0)$ and thus it can be shown that the first moments vanish while the second moments have the following asymptotic form for large $\tau$

$$\mu_2(\tau),\ \bar{\mu}_2(\tau) \approx FL\tau \qquad \text{when } \tau \to \infty \tag{41}$$

A similar analysis applied to the Fickian dispersion equation

$$\frac{\partial\gamma}{\partial\tau} - \frac{1}{Pe_t}\frac{\partial^2\gamma}{\partial\eta^2} = 0$$

shows that

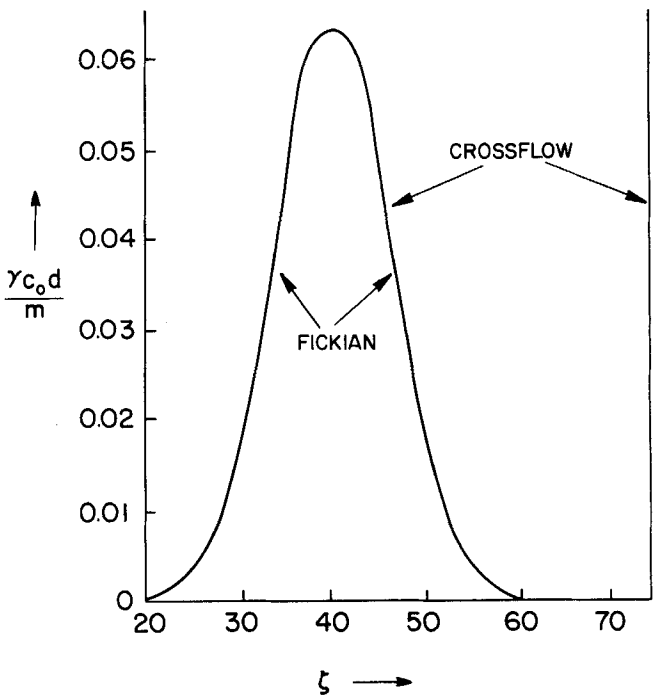


Figure 4. Pulse responses for Fickian and crossflow models. $\tau = 40$, $Pe_z = 2$, $S = 0.463$, $F = 0.429$.

$$\mu_2(\tau) \approx \frac{2\tau}{Pe_t} \qquad \text{when } \tau \to \infty \tag{42}$$

in this case. Thus, if the asymptotic rate of spreading, as measured by the second moment of the tracer concentration profile, is to be the same for both models, Equations (41) and (42) show that

$$Pe_t = \frac{2}{FL} \tag{43}$$

Equations (29) and (43) now identify both the parameters of the dimensionless Fickian dispersion model in terms of the parameters of the present model, in such a way that the rates of transverse and axial dispersion are the same for both models.

## EVALUATION OF THE MODEL PARAMETERS

The crossflow model is characterized by the three dimensionless parameters $S$, $F$ and $L$, defined by Equation (18). $L$ is given by $(\lambda/d)^2$, where $d$ is a characteristic dimension of the packing material and $\lambda$ is the scale of periodicity (in a statistical sense for a random packing) in the bed. Clearly $L$ will be a number of the order of unity, whose exact value will depend on the shape of the packing and the manner in which it was assembled to form the bed.

The remaining parameters, $S$ and $F$, are more difficult to obtain, but we now show that they can be estimated from experimental measurements of pressure drop and of the axial dispersion of an injected tracer pulse.

Consider first a steady flow of fluid through the bed in the direction of the $z$-axis, and focus on a slice of thickness $\delta z$ and unit cross-sectional area normal to this axis. Within this elemental slice, the mass flux of fluid between the stagnant and flowing regions is $f\rho\delta z$. The fluid leaving the flowing region has momentum $v$ per unit mass in the axial direction, while that replacing it has zero momentum in this direction, so there is a net rate of loss of axial momentum from the flowing stream in this slice equal to $f\rho v\delta z$. This contributes to the pressure gradient in the fluid, and if its contribution is denoted by $(dp/dz)'$ a momentum balance on the flowing fluid in the slice gives

$$-\epsilon_a(dp/dz)'\delta z = f\rho v\delta z$$

whence

$$-(dp/dz)' = \frac{f\rho v}{\epsilon_a} = \frac{f\rho\bar{u}}{\epsilon_a^2} \tag{44}$$

Now a number of equations have been proposed for the pressure drop in fluid flowing through a packed bed, for example the Ergun equation

$$-dp/dz = \frac{150\mu(1-\epsilon)^2\bar{u}}{\epsilon^3 d^2} + 1.75\left(\frac{1-\epsilon}{\epsilon^3}\right)\frac{\rho\bar{u}^2}{d} \tag{45}$$

in which $d$ denotes $6/S_v$, with $S_v$ equal to the ratio of surface area to volume for the packing material. Physically, the second term on the right hand side of the Ergun equation represents the contribution to the pressure gradient due to processes similar to the exchange of fluid between the flowing stream and "wakes" of relatively stagnant fluid. Thus it is reasonable to identify $-(dp/dz)'$, as given by Equation (44), with this term, and hence we find

$$\frac{fd}{\bar{u}} = 1.75\left(\frac{\epsilon_a}{\epsilon}\right)^2\frac{1-\epsilon}{\epsilon}$$

or

$$F = 1.75\,(1-S)^2\,\frac{1-\epsilon}{\epsilon} \tag{46}$$

giving a relation between $F$ and $S$. A second relation is provided by measured rates of axial dispersion, since Equation (29) shows that

$$F = S^2 Pe_z \tag{47}$$

and Equations (46) and (47) can easily be solved for $S$, with the result

$$\frac{S}{1-S} = \sqrt{\frac{1.75}{Pe_z}\left(\frac{1-\epsilon}{\epsilon}\right)} \tag{48}$$

Using this value for $S$, $F$ then follows from Equation (47).

The literature contains many measurements of effective axial Peclet numbers, and these indicate a rather weak dependence on Reynolds number in the range 10→500. However, the geometry of the packing material has a significant influence on the value of $Pe_z$, so a value corresponding to the type of packing of interest must be used in Equation (48) when evaluating $S$.

The weak dependence of $Pe_z$ on Reynolds number implies, through Equation (48), that $S$ also varies little with Reynolds number. However, it must be remembered that Equation (48) results from identifying the pressure losses associated with fluid transfer between stagnant and flowing regions, with the second term in the Ergun equation. This may not be entirely justified, particularly at low values of the Reynolds number.

Equation (48) may be compared with an empirical relation proposed by Gauvin and Katta (1973), namely

$$S = A\,\frac{(\epsilon-0.2)\,(1-\epsilon)}{\epsilon} \tag{49}$$

where $A$ is a constant whose value depends on the geometry of the packing material.

The values of $L$, $F$ and $S$ may be used to predict the transverse Peclet number, and it is interesting to compare such predictions with measured values. For this purpose, experimental values of both axial and transverse Peclet numbers are needed for the same bed; packing geometry and void fraction also must be known. As an example, we take the measurements of McHenry and Wilhelm (1957) on a random packed bed of glass spheres (diameter 0.32 cm), with a void fraction $\epsilon = 0.388$. Observed values of $Pe_z$ are very close to 2, so Equation (48) gives $S = 0.540$ and hence, from Equation (47), $F = 0.584$. With $d/\lambda = \sqrt{2}$, $L = 0.5$, so Equation (43) predicts that $Pe_t = 6.85$. This compares with measured values of about 10 obtained by Bernard and Wilhelm (1950) for the radial Peclet number. Note that a relatively small adjustment in the value of $d/\lambda$, from $\sqrt{2}$ to 1.7, would bring $Pe_t$ into agreement with the observed value.

As a second example, consider the measurements of England and Gunn (1970) on a random packed bed of cylinders. The packing material had length and diameter both equal to 0.64 cm, the void fraction was 0.350 and observed values of $Pe_z$, once more, were very close to 2. From these figures, $S = 0.560$, $F = 0.628$, and hence $Pe_t = 3.184/L$. Observed values of the radial Peclet number were close to 7, and this corresponds to a value $L = 0.455$ or $d/\lambda = 1.483$, which is not unreasonable.

## MODELLING DISPERSION IN PACKED BED REACTORS

It is usual to model axial dispersion in a packed tubular reactor by including a Fickian dispersion term. In the absence of radial composition variations, the dimensionless concentration $\gamma_i$ of each reacting species then satisfies a differential equation, of the form

$$\frac{d\gamma_i}{d\zeta} - \frac{1}{Pe_z}\frac{d^2\gamma_i}{d\zeta^2} = \mathcal{R}_i(\underline{\gamma}) \tag{50}$$

where $\mathcal{R}_i$ denotes the dimensionless rate of production of species $(i)$ by chemical reaction and $\underline{\gamma}$ represents the set of all the dimensionless concentrations $\gamma_i$. The explicit form of the function $\mathcal{R}_i$ depends on the rate expressions, of course. Since Equation (50) is second-order in $\zeta$, two boundary conditions are needed to determine a solution. These are commonly taken to be

$$\gamma_i^0 - \gamma_i = -\frac{1}{Pe_z}\frac{d\gamma_i}{d\zeta} \text{ at } \zeta = 0 \tag{51}$$

and

$$d\gamma_i/d\zeta = 0 \text{ at } \zeta = Z \tag{52}$$

where $\gamma_i^0$ is the concentration of $i$ upstream of the reactor and Z is its dimensionless length. The first of these arises from a material balance at entry to the reactor. The second has, from time to time, sparked controversies, and various arguments have been advanced to support it.

Regardless of any questions about the physical applicability of Equations (50) → (52), any attempt to obtain their solution, even for an isothermal reactor and quite simple first-order rate equations, leads quickly to very heavy algebra and cumbersome final results. This is a consequence of the exit boundary condition (52), which must be imposed to determine a solution.

An alternative representation of axial dispersion is provided by the crossflow model developed here, which yields the following equations in place of (50):

$$\frac{d\gamma_i}{d\zeta} + F(\gamma_i - \bar{\gamma}_i) = (1-S)\mathcal{R}_i(\gamma) \tag{53}$$

$$F(\bar{\gamma}_i - \gamma_i) = S\mathcal{R}_i(\bar{\gamma}) \tag{54}$$

and the accompanying boundary conditions are simply

$$\gamma_i = \gamma_i^0 \text{ at } \zeta = 0 \tag{55}$$

Equations (53) are first-order in $\zeta$, and the initial conditions (55) determine a unique solution. The algebraic task of solving equations (53) → (55) is much easier than that posed by Equations (50) → (52), as will be demonstrated.

Consider the simple case of a single irreversible reaction of first order with just one reactant, whose dimensionless concentration is denoted by $\gamma$. The reaction rate per unit fluid volume is then $kc$, where $k$ is the velocity constant, and the corresponding dimensionless reaction rate is given by $\mathcal{R} = J\gamma$, where $J = dk/u = dk\epsilon/\bar{u}$ ($J$ is the Damköhler number $Da_I$). In this case, the equations of the crossflow model reduce to

$$\frac{d\gamma}{d\zeta} + F(\gamma - \bar{\gamma}) = -J(1-S)\gamma$$

$$F(\bar{\gamma} - \gamma) = -JS\bar{\gamma}$$

and it is easy to eliminate $\bar{\gamma}$ from these, giving the single differential equation

$$\frac{d\gamma}{d\zeta} + J\left[\frac{1+(1-S)JS/F}{1+JS/F}\right]\gamma = 0 \tag{56}$$

whose solution can be written down immediately

$$\gamma = \gamma^0 \exp\left[-J\zeta\left(\frac{1+(1-S)JS/F}{1+JS/F}\right)\right] \tag{57}$$

In the limit as $F \to \infty$, Equation (56) reduces to the differential equation of a plug flow reactor, and (57) reduces to its familiar exponential solution.

The differential equation describing the corresponding solution modelled as Fickian dispersion is

$$\frac{d^2\gamma}{d\zeta^2} - Pe\,\frac{d\gamma}{d\zeta} - JPe\gamma = 0 \tag{58}$$

with general solution

$$\gamma = Ae^{\lambda_1\zeta} + Be^{\lambda_2\zeta}$$

where

$$\lambda_1, \lambda_2 = \frac{Pe}{2}\left[1 \pm \sqrt{1 + \frac{4J}{Pe}}\right]$$

and the constants $A$ and $B$ are determined by boundary conditions (51) and (52), with the result

$$\gamma(Z) = \frac{\gamma^0(\lambda_2 - \lambda_1)}{\lambda_2\left(1 - \frac{\lambda_1}{Pe}\right)e^{-\lambda_1 Z} - \lambda_1\left(1 - \frac{\lambda_2}{Pe}\right)e^{-\lambda_2 Z}} \tag{59}$$

This is significantly more complicated and more difficult to obtain than Equation (57) for the crossflow model.

The true advantage of the crossflow model is seen in cases which are a little more complicated, for example, a sequence of irreversible first order reactions

$$A_0 \xrightarrow{k_0} A_1 \xrightarrow{k_1} A_2 \xrightarrow{k_2} \text{Products}$$

The algebra of this example is simplest when all the velocity constants are the same, $k_0 = k_1 = k_2 = k$. Then the differential equations describing the crossflow model are

$$\left.\begin{aligned} \frac{d\gamma_0}{d\zeta} + F(\gamma_0 - \bar{\gamma}_0) &= -J(1-S)\gamma_0 \\ F(\bar{\gamma}_0 - \gamma_0) &= -JS\bar{\gamma}_0 \end{aligned}\right\} \tag{60}$$

and

$$\left.\begin{aligned} \frac{d\gamma_i}{d\zeta} + F(\gamma_i - \bar{\gamma}_i) &= J(1-S)(\gamma_{i-1} - \gamma_i) \\ F(\bar{\gamma}_i - \gamma_i) &= JS(\bar{\gamma}_{i-1} - \bar{\gamma}_i) \end{aligned}\right\} \; i = (1,2) \tag{61}$$

with initial conditions

$$\gamma_0(0) = \gamma_0^0;\ \gamma_i(0) = 0 (i = 1,2) \tag{62}$$

This initial value problem is not difficult to solve, with the result

$$\gamma_0 = \gamma_0^0 \exp(-X\zeta) \tag{63}$$

$$\gamma_1 = \gamma_0^0 J(1-S)\zeta\left[1 + \frac{S/(1-S)}{(1+JS/F)^2}\right]\exp(-X\zeta) \tag{64}$$

$$\gamma_2 = \gamma_0^0 J(1-S)\zeta\left\{\frac{(JS/F)(S/1-S)}{(1+JS/F)^3} + \frac{1}{2}J(1-S)\zeta\left[1+\frac{S/(1-S)}{(1+JS/F)^2}\right]^2\right\}\exp(-X\zeta) \tag{65}$$

where

TABLE 1. EXIT CONCENTRATIONS FOR $A_0 \to A_1 \to A_2 \to$ PROD. $\gamma_i(P)$ – PLUG FLOW MODEL; $\gamma_i(F)$ – FICKIAN MODEL; $\gamma_i(C)$ – CROSSFLOW MODEL.

| Z | $\gamma_0(P)$ | $\gamma_0(F)$ | $\gamma_0(C)$ | $\gamma_1(P)$ | $\gamma_1(F)$ | $\gamma_1(C)$ | $\gamma_2(P)$ | $\gamma_2(F)$ | $\gamma_2(C)$ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.8251 | 0.8330 | 0.8379 | 0.1587 | 0.1448 | 0.1375 | 0.0153 | 0.0194 | 0.0202 |
| 2 | 0.6807 | 0.6977 | 0.7020 | 0.2618 | 0.2359 | 0.2304 | 0.0503 | 0.0534 | 0.0528 |
| 4 | 0.4634 | 0.4900 | 0.4928 | 0.3564 | 0.3258 | 0.3235 | 0.1371 | 0.1290 | 0.1272 |
| 6 | 0.3154 | 0.3441 | 0.3460 | 0.3639 | 0.3413 | 0.3406 | 0.2100 | 0.1916 | 0.1898 |
| 8 | 0.2147 | 0.2417 | 0.2429 | 0.3303 | 0.3187 | 0.3188 | 0.2541 | 0.2313 | 0.2300 |
| 10 | 0.1462 | 0.1697 | 0.1705 | 0.2811 | 0.2793 | 0.2797 | 0.2703 | 0.2485 | 0.2477 |
| 12 | 0.0995 | 0.1192 | 0.1197 | 0.2296 | 0.2351 | 0.2357 | 0.2649 | 0.2477 | 0.2474 |
| 14 | 0.0677 | 0.0837 | 0.0840 | 0.1823 | 0.1925 | 0.1930 | 0.2455 | 0.2343 | 0.2342 |
| 16 | 0.0461 | 0.0588 | 0.0590 | 0.1419 | 0.1544 | 0.1548 | 0.2182 | 0.2132 | 0.2133 |
| 18 | 0.0314 | 0.0413 | 0.0414 | 0.1086 | 0.1219 | 0.1223 | 0.1880 | 0.1883 | 0.1886 |
| 20 | 0.0214 | 0.0290 | 0.0291 | 0.0822 | 0.0951 | 0.0954 | 0.1580 | 0.1625 | 0.1627 |

$$X = J\left[\frac{1 + (1-S)JS/F}{1 + JS/F}\right]$$

The corresponding differential equations for the Fickian model of this reactor are

$$\frac{d^2\gamma_0}{d\zeta^2} - Pe\frac{d\gamma_0}{d\zeta} - JPe\gamma_0 = 0 \qquad (66)$$

$$\frac{d^2\gamma_i}{d\zeta^2} - Pe\frac{d\gamma_i}{d\zeta} - JPe(\gamma_i - \gamma_{i-1}) = 0 \quad (i = 1,2) \qquad (67)$$

with associated boundary conditions

$$\gamma_0^0 - \gamma_0 = -\frac{1}{Pe}\frac{d\gamma_0}{d\zeta}(\zeta = 0); \frac{d\gamma_0}{d\zeta} = 0\,(\zeta = Z) \qquad (68)$$

and

$$\gamma_i = \frac{1}{Pe}\frac{d\gamma_i}{d\zeta}(\zeta = 0); \frac{d\gamma_i}{d\zeta} = 0\,(\zeta = Z)\,(i = 1,2) \qquad (69)$$

The solution of this problem is too cumbersome even to write out in digestably compact form. The reader who has any doubt regarding the relative simplicity of the crossflow model is recommended to attempt the explicit solution of Equations (66)-(69) and compare the volume of algebra generated with the results (63)→(65) above, from the differential equations of the crossflow model.

Table 1 compares the solutions of this sequential first-order reaction problem for the plug flow reactor, for a reactor with axial dispersion described by the Fickian model, and for the same reactor with dispersion described by the crossflow model. The values selected for the parameters of the crossflow model are $S = 0.4800$, $F = 0.4615$ and $J = 0.1923$. The corresponding value of the Peclet number given by Equation (29) is 2, and this was used in the calculations for the Fickian model.

The table gives the values of the dimensionless concentrations of $A_0$, $A_1$ and $A_2$ at the exit of reactors of various lengths from $Z = 1$ to $Z = 20$. Both dispersive models give results which differ significantly from the plug flow model, but there is little difference between the numerical predictions of the Fickian model and the crossflow model. There therefore appears to be little justification for using the Fickian model to describe axial dispersion in packed tubular reactors, in view of the much simpler mathematical problem posed by the crossflow model.

With nonlinear rate expressions, the equations describing both models must usually be solved numerically. Here again, the crossflow model is superior since it poses only an initial value problem for a set of simultaneous first-order ordinary differential equations, in contrast to the two-point boundary value problems generated by the Fickian model.

## NOTATION

$A$ = proportionality constant in Gauvin and Katta's equation
$\underline{c}$ = local average concentration in flowing region
$c$ = local average concentration in stagnant region
$c_0$ = concentration in stream entering bed
$d$ = length characteristic of packing material
$D_t$ = transverse dispersion coefficient
$D_z$ = axial dispersion coefficient
$f$ = volumetric exchange rate of fluid between stagnant and flowing regions, per unit bed volume
$F$ = $df/u$, dimensionless measure of $f$
$J$ = $dk/u$, Damköhler number $Da_I$
$k$ = velocity constant of chemical reaction
$L$ = $(\lambda/d)^2$, square of dimensionless layer spacing in bed
$m$ = amount of injected tracer per unit bed cross-section
$Pe_t$ = $ud/D_t$, transverse Peclet number
$Pe_z$ = $ud/D_z$, axial Peclet number
$R$ = rate of chemical reaction per unit fluid volume
$\mathcal{R}$ = $dR/uc_0$, dimensionless chemical reaction rate
$S$ = $\epsilon_b/\epsilon$, volume fraction of fluid regarded as stagnant
$S_v$ = ratio of surface area to volume for packing material
$\underline{u}$ = interstitial average fluid velocity in bed
$u$ = $\epsilon u$, superficial average fluid velocity in bed
$v$ = local average velocity of fluid in regions regarded as flowing
$x,y$ = co-ordinates measured perpendicular to direction of fluid flow
$z$ = co-ordinate measured in direction of fluid flow
$Z$ = dimensionless length of bed

### Greek Letters

$\alpha$ = fraction of stagnant fluid entering flowing stream in same layer
$\beta$ = fraction of flowing fluid entering stagnant regions in same layer
$\underline{\gamma}$ = $\underline{c}/c_0$, dimensionless concentration in flowing fluid
$\gamma$ = $c/c_0$, dimensionless concentration in stagnant fluid
$\epsilon$ = void fraction in bed
$\epsilon_a$ = volume occupied by flowing fluid, per unit bed volume
$\epsilon_b$ = volume occupied by stagnant fluid, per unit bed volume
$\zeta$ = $z/d$, dimensionless co-ordinate in direction of fluid flow
$\eta$ = $y/d$, dimensionless co-ordinate normal to direction of fluid flow
$\lambda$ = layer thickness in packed bed
$\mu$ = viscosity of fluid
$\xi$ = $x/d$, dimensionless co-ordinate normal to direction of fluid flow
$\rho$ = density of fluid
$\tau$ = $ut/d$, dimensionless time

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