Wave Model for Longitudinal Dispersion: Analysis and Applications

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An analysis and applications of the wave model for longitudinal dispersion are presented. Asymptotic forms of the wave model are considered and analytical solutions of typical linear stationary and nonstationary problems of chemical reactor engineering interest are obtained and compared to those for the Fickian dispersion model. The wave model leads to efficient analytical solutions for linear problems, which in principle differ from the solutions of the Fickian dispersion model; only for slowly varying concentration fields do the solutions of both models approach each other. Spatial and time moments of the concentration distribution are obtained for pulse-dispersion problems; the first three spatial moments of the mean, variance, and skewness have exact, large-time asymptotic forms in the case of Taylor dispersion. Old experiments that could not be explained with the standard dispersion model are reconsidered and explained: the change with time of the variance of a concentration pulse when the flow direction is reversed and the difference in values of the apparent axial dispersion coefficient and the backmixing coefficient in a rotating disk contactor. The experimental determination of model parameters is discussed.

Introduction

Many processes of interest in chemical engineering are analyzed in terms of transport equations for concentrations that are in some way averaged or in terms of what are referred to as dispersion equations. For mass- or heat-dispersion fluxes simple gradient laws like Fick's law for diffusion are commonly used. The most widespread model is the one-dimensional dispersed-plug-flow model or standard dispersion model (SDM) for a concentration averaged over the cross section to the flow. The shortcomings of this model are well known (see Westerterp et al., 1995). In the cited article the mathematical description of the way in which substances are dispersed along a channel, through which fluid flows in steady motion, has been reconsidered. As an alternative to the Fickian-type dispersion model and on the basis of two different approaches, a hyperbolic system of two first-order equations for the average concentration c and the dispersion flux j was obtained:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + \frac{\partial j}{\partial x} + q(c,x,t) = 0 \tag{1}$$

$$[1+\tau q'(c,x,t)]j + \tau\frac{\partial j}{\partial t} + \tau(u+u_a)\frac{\partial j}{\partial x} = -D_e\frac{\partial c}{\partial x} \tag{2}$$

where D_e, τ, and u_a are the parameters of the wave model (see Westerterp et al., 1995). For a first-order chemical reaction with a position-independent rate constant, Eqs. 1 and 2 become one second-order hyperbolic equation

$$\frac{\partial^2 c}{\partial t^2} + (2u+u_a)\frac{\partial^2 c}{\partial x\partial t} + (u^2+uu_a-D_e/\tau)\frac{\partial^2 c}{\partial x^2} + (\tau^{-1}+2k)\frac{\partial c}{\partial t} + [u/\tau + k(2u+u_a)]\frac{\partial c}{\partial x} + k(\tau^{-1}+k)c = 0. \tag{3}$$

The wave model of Eqs. 1 and 2 does not contain the conceptual deficiencies of the SDM. It also leads to a better under-

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standing of the mechanisms responsible for the characteristics of longitudinal dispersion phenomena.

The question arises: What does the application of the wave model give from a practical point of view and how does it interrelate to the SDM? There have been a number of papers setting up similar, mostly heuristic, models that are rarely compared with experiments. Therefore the general properties of the wave model and its potential benefits are treated here. The wave model will also be applied to several problems of interest to the chemical reactor or process engineering in order to demonstrate the essential advantages of the wave model over the SDM.

The asymptotic forms of the wave model and the conditions under which plug flow and ideal mixing are attained are considered. The analytical solutions of the linear stationary problem and the solutions of two nonstationary problems with an initial concentration pulse specified at some moment of time and at some point are obtained and compared with those of the Fickian dispersion model. For the linear problem the analytical solutions of the equations are as simple as for the Fickian dispersion model. The solutions differ fundamentally; only in slowly varying concentration fields are both models close to each other. Spatial and time moments of the concentration distribution are obtained; the first three spatial moments—mean, variance, and skewness—have exact long-term asymptotic forms in the case of Taylor dispersion. Two experimental studies are considered that cannot be explained with the SDM: the change over time of the variance of a concentration pulse, when the flow direction is reversed, and the difference in values of the apparent axial dispersion coefficient and the backmixing coefficient in a rotating disk contactor.

Asymptotic Forms of the Wave Model

For an analysis of the asymptotic forms of the wave model it is expedient to rewrite Eqs. 1 and 2 in dimensionless form:

$$\frac{\partial C}{\partial \theta}+\frac{\partial C}{\partial X}+\frac{\partial J}{\partial X}+Q(C,\theta,X)=0 \tag{4}$$

$$(P+Q')J+\frac{\partial J}{\partial \theta}+(1+u_a^*)\frac{\partial J}{\partial X}=-D_e^*\frac{\partial C}{\partial X} \tag{5}$$

where

$$C=\frac{c}{c_{ch}};\quad J=\frac{j}{uc_{ch}};\quad \theta=\frac{t}{t_{ch}};\quad X=\frac{x}{ut_{ch}};\quad P=\frac{t_{ch}}{\tau}$$

$$u_a^*=\frac{u_a}{u};\quad D_e^*=\frac{D_e}{u^2\tau};\quad Q=\frac{qt_{ch}}{c_{ch}}$$

and prime denotes derivative to the dimensionless concentration $Q'=dQ/dC$ and c_{ch} is the characteristic concentration. To be able to evaluate the relative contribution of each term in Eqs. 4 and 5, the characteristic time of the process t_{ch} must characterize the time of concentration changes. It depends, of course, on the problem under consideration. For example, for the stationary process in a chemical reactor it is the characteristic time of the chemical reaction; for a nonstationary tracer propagation it is the average residence time; and for steady periodic processes it is the cycle period.

From Eqs. 4 and 5 it follows that the dispersion flux can be neglected when the characteristic time t_{ch} is much larger than the relaxation time τ or $P \gg 1$: the wave model transforms into the plug-flow model:

$$\frac{\partial C}{\partial \theta}+\frac{\partial C}{\partial X}+Q(C,X,\theta)=0.$$

In the opposite case of $P \to 0$ we will restrict ourselves to the linear problem, assuming first-order kinetics with $q=kc$ where k is constant. We do so to avoid the difficulties in representing the consumption rate q through the average concentration c. In this limiting case Eqs. 4 and 5 transform into

$$\frac{\partial^2 C}{\partial \theta^2}+(2+u_a^*)\frac{\partial^2 C}{\partial X\partial\theta}+(1+u_a^*-D_e^*)\frac{\partial^2 C}{\partial X^2}+2Da\frac{\partial C}{\partial \theta}$$
$$+Da(2+u_a^*)\frac{\partial C}{\partial X}+Da^2C=0$$

where $Da=kt_{ch}$ is the Damköhler number. This equation can be reduced to

$$\frac{\partial^2 V}{\partial \theta^2}+(2+u_a^*)\frac{\partial^2 V}{\partial X\partial\theta}+(1+u_a^*-D_e^*)\frac{\partial^2 V}{\partial X^2}=0$$

by substituting $C=V\exp(-Da\theta)$. Introducing new variables $\omega_1=X-u_1^*\theta$ and $\omega_2=X-u_2^*\theta$, we arrive at the normal form of the hyperbolic equation

$$\frac{\partial^2 V}{\partial\omega_1\partial\omega_2}=0$$

where $u_{1,2}^*=1+(u_a^*/2)(1\pm\sqrt{1+4D_e^*/u_a^{*2}})$ are the dimensionless wave velocities. From this equation it follows that the most general solution of the problem under consideration is in the form of the sum of two waves that are damped by the chemical reaction:

$$C=f_1(\omega_1)e^{-Da\theta}+f_2(\omega_2)e^{-Da\theta}$$

where f_1 and f_2 can be any functions of ω_1 and ω_2, respectively. The obtained equation and its solution show that in the limiting case $t_{ch} \ll \tau$ the wave model corresponds to a linear combination of two plug-flow models with velocities equal to the wave velocities.

The wave model also transforms into the plug-flow model for sufficiently small values of the parameter of velocity asymmetry u_a^* and the dispersion coefficient D_e^* at fixed values of P. Actually from the definition of these parameters (see Westerterp et al., 1995) it follows that $D_e^* \to 0$ and $u_a^* \to 0$ when, as expected, the dispersion velocities of the longitudinal mixing process, or the wave velocities in a coordinate system moving with the average velocity, approach zero. This means the longitudinal velocity distribution approaches a uniform velocity profile. In this case the initial and boundary values of the dispersion flux are equal to zero, and the dispersion flux is always equal to zero due to Eq. 5. In the opposite case of large values of D_e^* and fixed values of u_a^* we may expect ideal mixing conditions. Note that in the general case the parameters of the wave model can have arbitrary values. But such a situation is impossible for Taylor dispersion in a unidirectional flow system, because longitudinal and transverse mixing are interrelated and the longitudinal dispersion coefficient D_e^* cannot exceed the value of $1+u_a^*$ in this case (Westerterp et al., 1995). The more general problem of independent longitudinal and transverse mixing—similar to the generalization of Taylor's theory made by Aris (1956)—must be considered if we desire to obtain the ideal mixing model as a limit in this case.

Relaxation of the Dispersion Flux

To study the properties of the wave model let us assume that the local concentration in a vessel does not depend on the longitudinal coordinate x, but does depend on the transverse coordinate. If we are interested in the phenomena in the central part of a sufficiently long reactor where the effect of the boundaries is insignificant, it is possible to consider the problem for an infinite region with initial conditions only. For this case the initial conditions are

$$t=0 \quad c=c_{\text{in}}, \quad j=j_{\text{in}},$$

and these initial values of the concentration and the dispersion flux are independent of the longitudinal coordinate x. The solution of Eqs. 1 and 2 for the case of no reaction is

$$c=c_{\text{in}}, \quad j=j_{\text{in}}e^{-t/\tau}.$$

This simple example shows that in contrast to SDM the dispersion flux is a variable independent of the concentration and that the relaxation time τ characterizes how quickly the system approaches the steady state.

Apparatus with Dispersion and Reaction in the Steady State

A good understanding of many of the issues involved can be developed from the study of linear problems. Accordingly, we start with a first-order irreversible chemical reaction and unidirectional flow. For that case, solutions for different initial and boundary conditions can be obtained analytically. The equation for the average concentration in the stationary state can conveniently be written in dimensionless form as

$$\alpha(1+u_a^*-D_e^*)\frac{d^2C}{dX^2}+(1+2\alpha+\alpha u_a^*)\frac{dC}{dX} + (1+\alpha)C=0 \qquad (6)$$

with the boundary conditions:

$$X=0, \quad C=\beta,$$

$$\frac{dC}{dX}=-\frac{(1+u_a^*)\beta-(1-\beta)(1+\alpha^{-1})}{1+u_a^*-D_e^*}=-\Lambda \qquad (7)$$

where $X=x/(ut_{ch})=kx/u$, $\alpha=k\tau$, $\beta=c_0/c_{b0}$, and c_{b0} is the bulk average concentration in the inlet stream; the characteristic time in this case is $t_{ch}=1/k$. The dimensionless dispersion flux at the reactor inlet is equal to $J=j_0/(uc_{b0})=1-\beta$, so the value of β characterizes the nonuniformity of the transverse concentration distribution at the reactor inlet. For a uniform concentration distribution at the inlet $\beta=1$.

The bulk average concentration $c_b=(cu+j)/u$, in dimensionless form $C_b=c_b/c_{b0}$, also obeys Eq. 6, but with different boundary conditions:

$$X=0, \quad C_b=1; \quad \frac{dC_b}{dX}=-\beta. \qquad (8)$$

The SDM in the chosen variables has the form:

$$-\alpha D_e^*\frac{d^2C_s}{dX^2}+\frac{dC_s}{dX}+C_s=0 \qquad (9)$$

$$X=0, \quad C_s-\alpha D_e^*\frac{dC_s}{dX}=1, \quad X=X_L, \quad \frac{dC_s}{dX}=0. \qquad (10)$$

The essential difference between the wave model and SDM is obvious. In the case of unidirectional flow the coefficients of the first and second derivatives in Eq. 6 are of the same sign, and both boundary conditions for this equation are set up at the inlet of the reactor, whereas in Eq. 9 the signs of these coefficients are opposed to each other. Moreover, the wave model does not contain the length of the reactor, the SDM does so in X_L. This fundamental difference is important from the physical point of view, and from the mathematical point of view it becomes very important for nonlinear problems as well as for multivariable linear problems, where a numerical solution is necessary.

It is interesting to compare the solutions of the wave model and the SDM for the problem considered. The solution of Eq. 6 with boundary conditions, Eq. 7, is

$$C=\frac{\Lambda+\beta\gamma_2}{\gamma_2-\gamma_1}e^{\gamma_1 X}-\frac{\Lambda+\beta\gamma_1}{\gamma_2-\gamma_1}e^{\gamma_2 X} \qquad (11)$$

where γ_1 and γ_2 are the roots of the equation

$$\alpha(1+u_a^*-D_e^*)\gamma^2+(1+2\alpha+\alpha u_a^*)\gamma+1+\alpha=0.$$

The distribution of the bulk average concentration along the reactor has the same form:

$$C_b=\frac{\beta+\gamma_2}{\gamma_2-\gamma_1}e^{\gamma_1 X}-\frac{\beta+\gamma_1}{\gamma_2-\gamma_1}e^{\gamma_2 X}. \qquad (12)$$

The solution of Eq. 9 with the boundary conditions, Eq. 10, is

$$C_s=\frac{\delta_1 e^{\delta_2(X-X_L)}-\delta_2 e^{\delta_1(X-X_L)}}{\delta_1(1-\alpha D_e^*\delta_2)e^{-\delta_2 X_L}-\delta_2(1-\alpha D_e^*\delta_1)e^{-\delta_1 X_L}} \qquad (13)$$

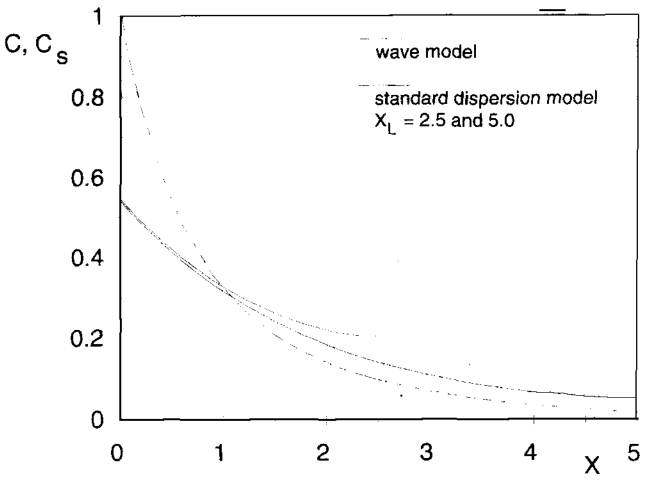


Figure 1. Concentration profiles for a first-order reaction calculated with the wave model and the standard dispersion model.

Model parameters: $D_e^* = 5/16$, $u_a^* = 1/4$, $\alpha = 5$.

where

$$\delta_{1,2} = \frac{1 \pm (1 + 4\alpha D_e^*)^{1/2}}{2\alpha D_e^*}.$$

The bulk average concentration for the SDM is expressed through the area average concentration by the equation

$$C_{sb} = C_s - \alpha D_e^* \frac{dC_s}{dX}. \tag{14}$$

The qualitative difference of the concentration distributions given by the wave model and the SDM for reactors of two different lengths is shown in Figure 1. The values of the parameters chosen for the calculations of $D_e^* = 5/16$ and $u_a^* = 1/4$ correspond to the well-developed laminar flow in a straight round tube.

The solutions of the wave model and the SDM are considered below for limiting values of the dimensionless chemical reaction rate α. For practical purposes the values of interest of X do not exceed 6 to 8, and therefore all asymptotic solutions below are given for the case when X is bounded. For a low reaction rate ($\alpha \to 0$) and fixed finite values of the model parameters it is easy to show that for a uniform concentration at the reactor inlet ($\beta = 1$) both models give the same results as the plug-flow model:

$$C = C_b \simeq C_s = C_{bs} = e^{-X}.$$

For a nonuniform inlet concentration distribution, the solutions of the two models also coincide except for a narrow region close to the inlet.

For fast reaction rates ($\alpha \to \infty$) the solutions are determined by Eqs. 11 to 14 with $\gamma_1 = -1/u_2^*$, $\gamma_2 = -1/u_1^*$, $\Lambda = [(u_1^* + u_2^*)\beta - 1]/(u_1^* u_2^*)$, and $\delta_{1,2} = \pm(\alpha D_e^*)^{-1/2}$. In this limiting case the SDM gives the following results, showing an incredible concentration dependence on the reactor length X_L:

$$C_s = \frac{1}{1 + X_L}, \quad C_{bs} = 1 - \frac{X}{1 + X_L}.$$

Note that for a reactor of semiinfinite length where $X_L \to \infty$ we have $c_s \to 0$ and $c_{bs} \to 1$. The corresponding solutions of the wave model for an inlet concentration distribution that is uniform over the cross section ($\beta = 1$) are

$$C = \frac{u_1^* - 1}{u_1^* - u_2^*} e^{-X/u_2^*} + \frac{1 - u_2^*}{u_1^* - u_2^*} e^{-X/u_1^*} \tag{15}$$

$$C_b = \frac{u_2^*(u_1^* - 1)}{u_1^* - u_2^*} e^{-X/u_2^*} + \frac{u_1^*(1 - u_2^*)}{u_1^* - u_2^*} e^{-X/u_1^*}. \tag{16}$$

Equations 15 and 16 show that for high reaction rates the wave-model limit corresponds to a combination of two plug-flow models with velocities equal to the wave velocities. These solutions differ noticeably from the ones for the SDM.

Analytical Solutions of the Wave Model for a Pulse Injection

For linear problems, analytical solutions of Eqs. 1 and 2, can be obtained for various initial and boundary conditions by standard methods, using, for instance, integral forms of solution (see Tikhonov and Samarskii, 1963) or Laplace transforms (see Aris and Amundson, 1973). Two of the typical pulse-response problems are presented below. For the sake of simplicity the component consumption rate q is assumed to be equal to zero, although for a first-order chemical reaction this does not influence the complexity of the solution. This can be seen after substituting $v\exp(-kt)$ for c in Eq. 3 and in the initial and boundary conditions, which reduces Eq. 3 to an equation for v without the reaction term.

Initial spatial distribution

First consider the solution for an amount M of material, released at time $t = 0$ and in the narrow x-axis region in the neighborhood of the point $x = 0$ uniformly over the cross section to the flow. The initial conditions for Eqs. 1 and 2 are

$$t = 0, \quad c = \frac{M}{A}\delta(x), \quad j = 0$$

where $\delta(x)$ is a Dirac delta function. The corresponding initial conditions for Eq. 3 are

$$t = 0, \quad c = \frac{M}{A}\delta(x), \quad \frac{\partial c}{\partial t} = -\frac{Mu}{A}\delta'(x)$$

where the prime denotes the derivative. The solution of Eq. 3 for an infinitely long domain is not equal to zero for $u_2 t \leq x \leq u_1 t$, and can be written as

$$c = \frac{M}{Au\tau} e^{-\beta_1\eta_2 - \beta_2\eta_1} \left\{ \frac{u_1 - u}{u_1 - u_2}\delta(\eta_2) + \frac{u - u_2}{u_1 - u_2}\delta(\eta_1) + pI_0(Y) + p(\beta_1\eta_1 + \beta_2\eta_2)\frac{I_1(Y)}{Y} \right\} \tag{17}$$

where I_0 and I_1 are modified Bessel functions of zero and first order, and

$$\eta_1 = \frac{u_1 t - x}{u\tau}, \quad \eta_2 = \frac{x - u_2 t}{u\tau}, \quad \beta_1 = \frac{(u_1 - u)u}{(u_1 - u_2)^2},$$

$$\beta_2 = \frac{(u - u_2)u}{(u_1 - u_2)^2}, \quad Y = 2(\beta_1 \beta_2 \eta_1 \eta_2)^{1/2},$$

$$p = \frac{2(u_1 - u)(u - u_2)u}{(u_1 - u_2)^3} = 2\beta_1 \beta_2 \frac{u_1 - u_2}{u}. \tag{18}$$

The obtained solution has two abrupt fronts at $x = u_1 t$ and $x = u_2 t$, where the concentration suddenly falls to zero. Using the asymptotic form for the modified Bessel functions for a sufficiently large time:

$$\frac{t}{\tau} \gg \frac{(u_1 - u_2)^2}{(u_1 - u)(u - u_2)} = 4 + \frac{u_a^2 \tau}{D_e}$$

and provided $|x - ut| \ll \min[(u_1 - u)t, (u - u_2)t]$, Eq. 17 develops into a Gaussian distribution of the concentration as a function of x with the mean ut and a variance $2D_e t$:

$$c = \frac{M}{A} \frac{1}{2\sqrt{\pi D_e t}} e^{-(x-ut)^2/4D_e t} \tag{19}$$

as is also given by the SDM for the initial condition $c = (M/A)\delta(x)$ at $t = 0$ and for the infinite region, where the effect of the boundaries is not significant. Thus the solution of the wave model coincides with the normal distribution only in the central part of the tracer cloud and only after a sufficiently long time.

Input concentration specified as a function of time

The next problem we wish to solve is the one where the concentration is specified as a function of time at some fixed point $x = 0$. Suppose that at the initial moment $t = 0$ the concentration is zero everywhere along the x-axis and that solute of an amount M is introduced at point $x = 0$ during a sufficiently short period of time and uniformly over the cross section to the flow. The initial and boundary conditions in this case for Eqs. 1 and 2 are

$$t = 0, \quad c = 0, \quad j = 0; \quad x = 0, \quad c = \frac{M}{Au}\delta(t), \quad j = 0.$$

The corresponding initial and boundary conditions for Eq. 3 are

$$t = 0, \quad c = 0, \quad \frac{\partial c}{\partial t} = 0; \quad x = 0, \quad c = \frac{M}{Au}\delta(t),$$

$$\frac{\partial c}{\partial x} = -\frac{M}{Au}\frac{u_1 + u_2 - u}{u_1 u_2}\delta'(t).$$

The solution of Eq. 3 for the problem is

$$c = \frac{M}{Au\tau} e^{-\beta_1\eta_2 - \beta_2\eta_1} \left\{ \frac{(u_1 - u)u_2}{(u_1 - u_2)u}\delta(\eta_2) + \frac{(u - u_2)u_1}{(u_1 - u_2)u}\delta(\eta_1) \right.$$

$$\left. + p\frac{u_1 + u_2}{2u} I_0(Y) + p\left(\beta_1\eta_1\frac{u_2}{u} + \beta_2\eta_2\frac{u_1}{u}\right)\frac{I_1(Y)}{Y} \right\}. \tag{20}$$

Equation 20, like Eq. 17, has the Gaussian asymptotic of Eq. 19 at the central part of the concentration distribution at the same conditions as for Eq. 17.

Equations 17 and 20 give similar concentration distributions. The characteristic features of these distributions are two concentration spikes in the front of the cloud of material, which are remnants of the initial and boundary conditions, respectively. Spikes in the form of δ-functions are unrealistic, but one should realize that they are the direct consequence of the two-velocity character of the simplest version of the wave model being considered. The positions of the spike and the quantities of substance in them correspond qualitatively to the double-peaked structure of known experimental results and numerical solutions for a short time (see Smith, 1981; Wang and Stewart, 1983, 1989; Korenaga et al., 1989; Takahashi et al., 1990). These concentration spikes were observed only at an early stage compared to the relaxation time of the dispersion. At a later stage in the dispersion process the amount of substance in the spikes becomes relatively small.

The obtained solutions give the residence time distributions of tracer for two different inputs that coincide after a sufficiently long time, but differ for short periods. The considered tracer inputs differ in the distribution of the amount of the substance introduced over the cross section or over the longitudinal velocity. In the first case, the distribution of a tracer over the cross section of the flow is uniform. In the second case, the tracer is injected in such a way that the amount introduced at some position is proportional to the velocity in this point, so the residence time distribution of tracer, Eq. 20, corresponds to the residence time distribution of the fluid elements. It is easy to prove that Eq. 20 predicts the conversion in a reactor with a first-order chemical reaction in a steady-state operation: the solution of Eq. 6 for a uniform input—Eq. 11 at $\beta = 1$—in dimensional form is equal to

$$c(x) = c_0 \int_0^\infty e^{-kt} E(x,t)\, dt$$

where $E(x, t)$ is the function determined by Eq. 20 at the coordinate $x = L$, that is, it is related to the residence time distribution of the fluid elements via a Laplace transform. The preceding result shows that the relation between the residence time distribution and conversion, which is well known for the SDM (see Westerterp et al., 1987), is also valid for the wave model, although with additional restrictions on material inputs.

Consideration of pulse-propagation problems on the basis of the wave model avoids the conceptual difficulties associated with material flow through "open" boundaries as we observe for the SDM (see Nauman, 1981 and Westerterp et al., 1987). The treatment of problems with initial and boundary conditions on the basis of the wave model differs only slightly from the treatment of limiting problems without boundary conditions, whereas consideration of the boundary conditions for a Fickian dispersion model makes the solution of the equations very difficult (see Novy et al., 1990).

Spatial and Temporal Moments

After the pioneering work of Aris (1956) the description of the distribution of a solute in terms of the moments of the concentration distribution has been widely used for the mathematical description of dispersion processes, since the moments of a cloud of solute are easier to calculate than the concentration distribution itself. Also knowledge of the first two or three moments of the concentration distribution gives much information about the concentration distribution itself (see Brenner, 1980, 1982; Brenner and Edwards, 1993). Models often are also compared by means of calculating the spatial—at a fixed moment of time—and the temporal—at a fixed coordinate location—moments of the concentration of an injected solute.

The spatial and temporal moments can easily be calculated by means of the proposed wave model by standard methods when the distribution of the concentration c at time $t = 0$ or at longitudinal position $x = 0$ is known. As an example, spatial moments of concentration around the mean are introduced:

$$\mu_n = \frac{\int_{-\infty}^{\infty} (x - \bar{x})^n c\, dx}{m}; \quad n = 2, 3, \ldots \tag{21}$$

where

$$\bar{x} = \frac{\int_{-\infty}^{\infty} xc\, dx}{m}; \quad m = \frac{M}{A} = \int_{-\infty}^{\infty} c\, dx. \tag{22}$$

The expressions for the first three moments are given below for the case of an arbitrary concentration distribution at $t = 0$ and a finite mass of solute:

$$\bar{x} = ut + \lambda_0 \tau (1 - e^{-\xi}) \tag{23}$$

$$\mu_2 = \mu_{2,\mathrm{in}} + 2\tau(\lambda_1 + \tau u_a \lambda_0 - D_e)(1 - e^{-\xi}) + 2\tau\xi(D_e - \tau u_a \lambda_0 e^{-\xi}) \tag{24}$$

$$\begin{aligned}\mu_3 = \mu_{3,\mathrm{in}} &+ 3\tau(\lambda_2 - \mu_{2,\mathrm{in}}\lambda_0)(1 - e^{-\xi}) + 2\lambda_0^3\tau^3(1 - e^{-\xi})^3 \\ &- \lambda_0\lambda_1\tau^2(1 - e^{-\xi})^2 + 6u_a\lambda_0^2\tau^3(1 - e^{-\xi})(\xi e^{-\xi} - 1 + e^{-\xi}) \\ &+ 6D_e\lambda_0\tau^2(2\xi e^{-\xi} - 1 + e^{-2\xi}) \\ &+ 6u_a\tau^2[(\lambda_1 + u_a\tau\lambda_0)(1 - \xi e^{-\xi} - e^{-\xi}) \\ &+ D_e(\xi + \xi e^{-\xi} + 2e^{-\xi} - 2) - u_a\tau\lambda_0(\xi^2/2)e^{-\xi}]\end{aligned} \tag{25}$$

where $\xi = t/\tau$ and $\mu_{n,\mathrm{in}}$ and λ_n are the initial values of the concentration and dispersion flux moments in a coordinate system chosen such that $\bar{x} = 0$ at $t = 0$:

$$\mu_{n,\mathrm{in}} = \frac{\int_{-\infty}^{\infty} x^n c_{\mathrm{in}}(x)\, dx}{m} \quad \lambda_n = \frac{\int_{-\infty}^{\infty} x^n j_{\mathrm{in}}(x)\, dx}{m}, \quad n = 0, 1, 2, \ldots. \tag{26}$$

After a small time t just after injection or $\xi \ll 1$, the moments are

$$\bar{x} = (1 + \lambda_0)ut \tag{27}$$

$$\mu_2 = \mu_{2,\mathrm{in}} + 2\lambda_1 t + (u_a\tau\lambda_0 - \lambda_1 + D_e)t^2/\tau \tag{28}$$

$$\begin{aligned}\mu_3 = \mu_{3,\mathrm{in}} &+ (\lambda_2 - \mu_{2,\mathrm{in}}\lambda_0)t/\tau + 3\lambda_1(u_a - 2\lambda_0)t^2 \\ &+ (2\lambda_0 - 3u_a\lambda_0^2 - 2D_e\lambda_0/\tau + u_a D_e/\tau - 2\lambda_1 u_a/\tau + \lambda_0 u_a^2)t^3\end{aligned} \tag{29}$$

and asymptotic values of moments after a very large time or $\xi \gg 1$ are

$$\bar{x} = ut; \quad \mu_2 = 2D_e t; \quad \mu_3 = 6D_e u_a \tau t. \tag{30}$$

The mean and variance in Eq. 30 do not depend on the relaxation time, the parameter of velocity asymmetry, and the initial value of the dispersion flux; they are the same as predicted by the SDM. When the injected solute is initially uniform over the cross section to the flow, then $j_{\mathrm{in}}(x) = 0$, $\lambda_n = 0$ for $n = 0, 1, 2, \ldots$ and the expressions for the moments are essentially simplified:

$$\begin{aligned}\bar{x} = ut; \quad \mu_2 &= \mu_{2,\mathrm{in}} + 2\tau D_e(\xi - 1 + e^{-\xi}) \\ \mu_3 &= \mu_{3,\mathrm{in}} + 6D_e u_a \tau^2(\xi + \xi e^{-\xi} + 2e^{-\xi} - 2).\end{aligned} \tag{31}$$

The equations for the moments with respect to the coordinate x were first formulated by Aris (1956), who also found the asymptotic behavior of the second moment around the mean. After Aris this problem was investigated by Chatwin (1970). The most general results were obtained by Barton (1983), who derived the second and third moments for arbitrary values of time. The calculations of Barton for the third moment are restricted to the case where solute is injected initially uniformly over the cross section. Equation 25 gives the approximate value of the third moment for an arbitrary initial concentration. Using the expressions for D_e, τ, and u_a obtained in the previous paper (see Westerterp et al., 1995), it can be easily shown that Eqs. 30 coincide with the asymptotic expressions of the first three moments obtained by Barton (1983). At small and moderate values of time, Eqs. 23, 24, and 25 have the same qualitative structure as the exact equations. Note that application of the SDM for calculating spatial moments gives $\mu_2 = 2D_e t$ and $\mu_3 = 0$ for all moments of time.

It is interesting to note that Taylor (1921), in a classic paper on turbulent diffusion, written long before his 1953 papers on axial dispersion, found the law of dispersion of the form of Eq. 31 for μ_2.

The temporal or time moments of concentration at some point x also can be calculated easily from the wave model for different initial and boundary conditions. As an example the mean residence time and the variance at point x for a tracer input uniform over cross section are

$$\bar{t} = \frac{x}{u} + \frac{D_e(1 - e^{-\lambda\zeta})}{u^2} \tag{32}$$

$$\sigma_t^2 = \sigma_{t,0}^2 + 2\left(\frac{x}{u}\right)^2 \frac{D_e}{xu}\Bigg[\lambda(1 + D_e^*) + \left(\lambda(u_a^* - 2D_e^*) + \frac{3D_e^* - 1 - 2u_a^*}{\zeta}\right)(1 - e^{-\lambda\zeta}) - \frac{D_e^*}{2\zeta}(1 - e^{-2\lambda\zeta})\Bigg] \tag{33}$$

where $\sigma_{t,0}^2$ is the value of the variance at point $x = 0$; further, $\zeta = x/(u\tau)$ and $\lambda = (1 + u_a^* - D_e^*)^{-1}$. The mean residence time and variance in Eqs. 32 and 33 are determined by standard equations:

$$\bar{t} = \frac{\int_0^\infty tc\,dt}{m}; \quad \sigma_t^2 = \frac{\int_0^\infty (t - \bar{t})^2 c\,dt}{m}; \quad m = \frac{M}{A} = \int_0^\infty c\,dt, \tag{34}$$

and the origin on the x-axis is chosen such that $\bar{t} = 0$ at $x = 0$. At a sufficiently long distance from the point $x = 0$ or $\zeta \gg 1$ the mean residence time and variance approach those for the SDM:

$$\bar{t} = \frac{x}{u} + \frac{D_e}{u^2}$$

$$\sigma_t^2 = \sigma_{t,0}^2 + 2\left(\frac{x}{u}\right)^2 \frac{D_e}{xu}\left[1 + \frac{5}{2}\frac{D_e}{ux} - \frac{u\tau}{x}\left(1 + \frac{u_a}{u}\right)\right].$$

In the opposite limiting case of $\zeta \ll 1$, we have

$$\bar{t} = \frac{x}{u}\left(1 + \frac{D_e}{u(u + u_a)\tau - D_e}\right)$$

$$\sigma_t^2 = \sigma_{t,0}^2 + \left(\frac{x}{u}\right)^2\left(1 + \frac{D_e u^2 \tau}{(u(u + u_a)\tau - D_e)^2}\right).$$

The values obtained here differ essentially from those of the standard dispersion model.

Axial Mixing in a Rotating Disk Contactor

More than thirty years ago Westerterp and Landsman (1962) and Westerterp and Meyberg (1962) investigated the axial mixing in a rotating disk contactor for homogeneous liquid-phase operation. The rotating disk contactor (see Figure 2) is a column that is divided by equally spaced stator rings into a number of compartments. Half-way in the stator rings a number of disk rotors are mounted on a shaft, the diameter of the rotors being smaller than the inner diameter of the stator rings. Experimental results have been interpreted by means of a diffusion model. The axial dispersion coefficient was found from the response at the outlet of the column to a stepwise change in the inlet concentration of a tracer; this axial dispersion coefficient was called the apparent axial diffusivity D_a (see Westerterp and Landsman, 1962). The apparent axial diffusivity could be considered to be the sum of a flow contribution and a rotational contribution:

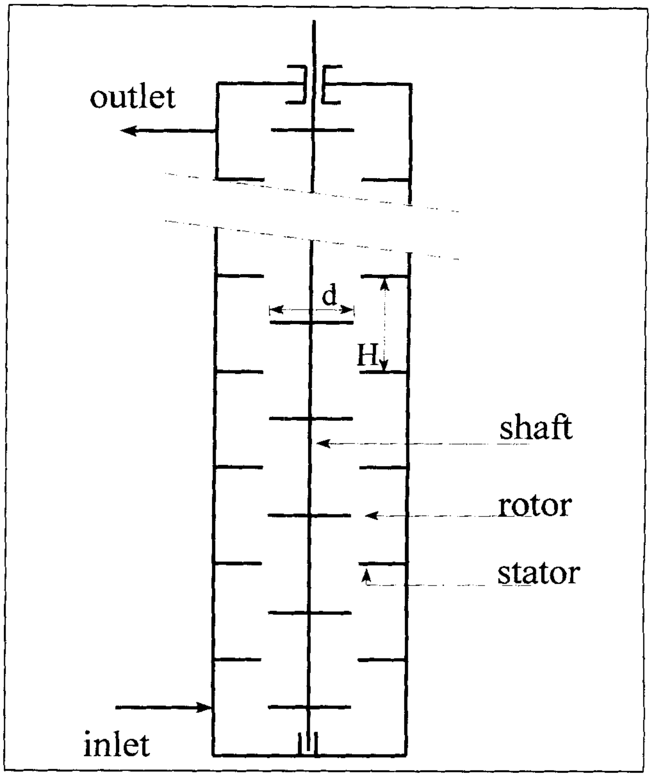


Figure 2. Rotating disk contactor.

$$D_a = \frac{1}{2}Hu + 13\cdot10^{-3}\frac{1}{2}Hnd, \quad \text{m}^2/\text{s} \tag{35}$$

where H is the height of a compartment in m, u is the average liquid velocity in m/s, n is the rotational speed in s^{-1}, and d the diameter of rotor in m. Also the true backmixing was measured under steady-state conditions, and the corresponding axial dispersion coefficient was called the backmixing coefficient, D_b (see Westerterp and Meyberg, 1962). The backmixing coefficient appeared to be equal to that part of the apparent axial diffusivity in Eq. 35 that is caused by the stirring, being $D_b = \text{const} \times Hnd$. The results of these two investigations cannot be reconciled by the SDM, since the axial dispersion coefficient depends on the experimental method. The same problem is known for dispersion in estuaries, where the apparent dispersion coefficient is a few times higher than the backmixing coefficient (see Fischer et al., 1979). Therefore we will interpret these experiments again by means of the wave model.

First let us consider the steady-state backmixing experiments. We are interested in the mixing in the central part of the column, where over a compartment averaged velocity remains constant along the column; therefore we can apply Eq. 3 for the steady state and with $q = 0$:

$$(\tau u^2 + \tau u u_a - D_e)\frac{d^2 c}{dx^2} + u\frac{dc}{dx} = 0. \tag{36}$$

If the tracer is injected at the plane $x = 0$ in the upper part of the column into the upward flowing fluid stream under steady-state conditions, some tracer will be found in the fluid upstream of the injection point at the locations with $x < 0$. This transport against the main flow of the fluid is caused by the fluid backflow caused by the stirring. The existence of a backflow in terms of the wave model means that the velocity of one of the waves, as well as the value of $\tau u^2 + \tau u u_a - D_e$, is negative in contrast to the case of unidirectional flow. This means that the boundary conditions for the central part of the column should be specified at both ends. For a sufficiently long column, as was used by Westerterp and Meyberg (1962), the boundary conditions are:

$$x = 0, \quad c = c_0; \quad x \to -\infty, \quad c \to 0.$$

The solution of Eq. 36 using these boundary conditions is

$$\frac{c}{c_0} = \exp\left(\frac{ux}{D_e - \tau u^2 - \tau u u_a}\right), \tag{37}$$

whereas the solution of the SDM, used by Westerterp and Meyberg is

$$\frac{c}{c_0} = \exp\left(\frac{ux}{D_b}\right). \tag{38}$$

Equations 37 and 38 show that the backmixing coefficient D_b measured by Westerterp and Meyberg is equal to $D_e - \tau u^2 - \tau u u_a$.

Let us now suppose that the relaxation time τ is much smaller than the mean residence time in the column. In that case the apparent axial diffusivity D_a, measured by Westerterp and Landsman (1962), is the axial dispersion coefficient of the wave model, D_e. Thus for the difference of the apparent diffusivity D_e and the backmixing coefficient D_b we can write

$$D_e - D_b = D_a - D_b = \tau u(u + u_a) = \frac{1}{2}Hu. \tag{39}$$

In the case of no net flow through the column, the rotating elements create an approximately symmetrical velocity distribution with respect to the cross section of the column. We can also expect that for low average velocities u used in experiments—relative to the velocities created by rotating disks—the violation of the symmetry of the tracer propagation in both the upflow and downflow directions is insignificant. In that case, $u_a \ll u$ and Eq. 39 gives the physically reasonable estimate of the relaxation time $\tau \approx (1/2)H/u$. The number of compartments in the column was $N = 24$. Therefore the relaxation time obtained is much lower than the mean residence time $t = NH/u$—as was supposed earlier—and the apparent diffusivity measured by Westerterp and Landsman (1962) is actually the axial dispersion coefficient of the wave model.

Flow reversal

An interesting effect was observed when the flow direction was reversed during a dispersion experiment. Such an investigation in a two-dimensional model of a packing of spheres was made by Hiby (1963); measurements in naturally occurring porous media have also been reported by Jasti and Fogler (1992). The spread in the spatial distribution narrows initially during a certain period of time after the flow direction has been reversed (see Figure 1 of Jasti and Fogler, 1992). The standard deviation of the tracer signal decreases upon flow reversal, whereas the local concentration of the tracer increases. The tracer again undergoes the typical dilution process after this initial period has passed. This example can be used to demonstrate the essential differences between the SDM and the wave model; it also helps to explain the essential properties of the wave model.

The equation describing the tracer distribution before the reversal of the flow direction is

$$\frac{\partial^2 c_1}{\partial t^2} + (2u + u_a)\frac{\partial^2 c_1}{\partial x \partial t} + (u^2 + u u_a - D_e/\tau)\frac{\partial^2 c_1}{\partial x^2} + \frac{1}{\tau}\left(\frac{\partial c_1}{\partial t} + u\frac{\partial c_1}{\partial x}\right) = 0, \quad 0 \le t \le t_R. \tag{40}$$

For simplicity we assume that initially the tracer was uniformly distributed over the cross section of the flow and is concentrated in a narrow region of the x-axis. In this case, $j = 0$ at $t = 0$, and the initial conditions for Eq. 40 are

$$t = 0, \quad c = c_0\delta(x), \quad \frac{\partial c}{\partial t} = -c_0\delta'(x). \tag{41}$$

At the moment, t_R, the flow direction is reversed, the signs of u and u_a change, and the governing equation transforms into:

$$\frac{\partial^2 c_2}{\partial t^2} - (2u + u_a)\frac{\partial^2 c_2}{\partial x \partial t} + (u^2 + u u_a - D_e/\tau)\frac{\partial^2 c_2}{\partial x^2} + \frac{1}{\tau}\left(\frac{\partial c_2}{\partial t} - u\frac{\partial c_2}{\partial x}\right) = 0, \quad t \ge t_R. \tag{42}$$

To specify the initial conditions for Eq. 42, we can use the assumption—justified in particular for liquids—that the concentration field does not change appreciably during the reversing of the flow. This means that at $t = t_R$ the average concentration is a continuous function of time, that is, $c_2 = c_1$, whereas the dispersion flux changes in sign, $j_2 = -j_1$. The mass conservation equations for $t \le t_R$ and for $t \ge t_R$ are

$$\frac{\partial c_1}{\partial t} + u\frac{\partial c_1}{\partial x} + \frac{\partial j_1}{\partial x} = 0, \quad 0 \le t \le t_R$$

$$\frac{\partial c_2}{\partial t} - u\frac{\partial c_2}{\partial x} + \frac{\partial j_2}{\partial x} = 0, \quad t \ge t_R.$$

From these equations and the conditions just mentioned at $t=t_R$, we find the initial conditions for Eq. 42:

$$t=t_R,\quad c_2=c_1,\quad \frac{\partial c_2}{\partial t}=-\frac{\partial c_1}{\partial t}. \tag{43}$$

The determination of the spatial moments of the concentration distribution from Eqs. 40 and 42 with the initial conditions Eqs. 41 and 43 is straightforward. Before the flow reversal, the moments of the spatial distribution are determined by Eq. 31. After the reversal, the mean and variance are

$$\bar{x}=u(2t_R-t) \tag{44}$$

$$\sigma_x^2=2D_e\tau\left[\frac{t}{\tau}-3+2e^{-t_R/\tau}+(2e^{t_R/\tau}-1)e^{-t/\tau}\right]. \tag{45}$$

Dependence on the time of the variance of the spatial distribution of the tracer is shown in Figure 3 for different reversing times t_R. The calculated results coincide qualitatively with those obtained experimentally by Jasti and Fogler (1992). A quantitative agreement between theory and the experiments of Jasti and Fogler can be obtained by the choice of parameters D_e and τ. Note that according to the SDM $\sigma_x^2=2D_et$, so the flow reversal does not influence the dependence of the variance on time.

The phenomenon considered is referred to as "unmixing" (see Jasti and Fogler, 1992). The physical reason for this phenomenon is known and easy to understand (see Hiby, 1963). After reversal, the concentration profile has to change, but a time of approximately τ is required before the concentration profile can completely adapt itself to the new velocity profile; immediately after reversing, the tracer molecules seem to retrace their flow paths and, as a consequence, the tracer pulse undergoes a concentrating process. The wave model is capable of describing this phenomenon, whereas the SDM is not.

From Eq. 45 we find that the spatial distribution narrows after reversing the flow during a period of time Δt:

$$\Delta t=\ln(2e^{t_R/\tau}-1)-t_R \tag{46}$$

and that the maximum decrease of the variance is

$$\Delta\sigma_{x,\max}^2=\sigma_x^2(t_R)-\sigma_x^2(t_R+\Delta t)$$
$$=2D_e\tau\left[\frac{t_R}{\tau}+1-e^{-t_R/\tau}-\ln(2e^{t_R/\tau}-1)\right]. \tag{47}$$

If flow reversal occurs at moments of time much smaller than the relaxation time or $t_R\ll\tau$, we find

$$\Delta t=t_R,\quad \Delta\sigma_{\max}^2=D_e\frac{t_R^2}{\tau}. \tag{48}$$

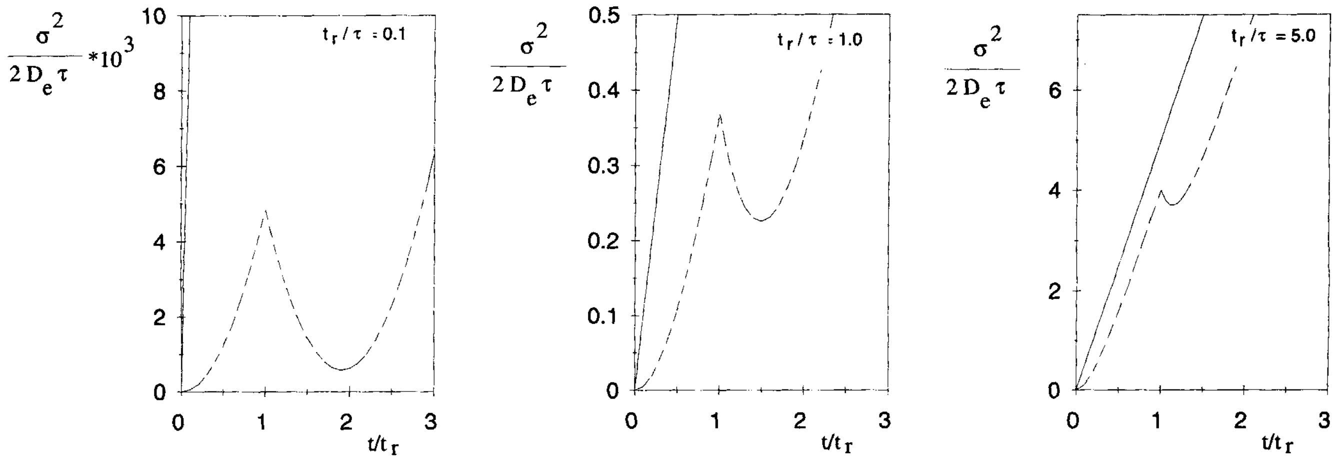
In the opposite case of $t_R\gg\tau$, then

$$\Delta t=\tau\ln 2,\quad \Delta\sigma_{x,\max}^2=2(1-\ln 2)D_e\tau. \tag{49}$$

The results for $t_R\ll\tau$ show that a purely convective, completely reversible contraction of the concentration cloud occurs after flow reversal during a period of time of the order of t_R (see Hiby, 1962).

Discussion

The use of hyperbolic-type equations for the description of different heat and mass dispersion phenomena was suggested a long time ago (see Stewart, 1965; Thacker, 1976; Maron, 1978; Smith, 1981). Such models did not receive much attention, however, probably because we are not accustomed to hyperbolic-type equations for dispersion processes. But physical considerations require that there should be finite velocity limits that are not exceeded by any fluid element, provided molecular diffusion is neglected. For this reason, from the physical point of view relaxation-type equations for dispersion fluxes should be preferred over Fickian-type dispersion



(a) **(b)** **(c)**

Figure 3. Effect of flow reversal on the variance of the tracer spatial distribution as calculated with the wave model (---) and the standard dispersion model (——).

(a)$t_r/\tau=0.1$; (b) $t_r/\tau=1.0$; (c)$t_r/\tau=5.0$.

equations. Moreover, almost all fields of science or engineering involve some questions of wave motion. Wave equations are used in acoustics, elasticity, and electromagnetism, and their basic properties and solutions were first studied in these areas of classical physics (see Whitham, 1974). Therefore applying the wave model to longitudinal dispersion does not create unresolved mathematical problems or unknown physics.

The main practical advantages of the wave model

Being physically more realistic than the SDM, the wave model is open to solutions for arbitrary linear problems. In contrast to the SDM, the mathematical complexity of the wave model does not depend essentially on the boundary and initial conditions for Eqs. 1 and 2. An important aspect of Eqs. 1 and 2 is that the boundary conditions—in contrast to those of the Fickian-type dispersion model—for unidirectional flow are set at the inlet only. This also gives rise to a considerable mathematical simplification of nonlinear problems as well as multicomponent and multivariable linear problems, where a numerical solution is necessary. Consequently, since it offers a more consistent physical picture than the Fickian dispersion model, the present model has a considerable advantage in computational efforts. The mathematical solutions of the wave model are simpler or as simple as for the SDM.

Physical contradictions in the SDM give rise to the problem of boundary conditions. As a consequence, a multiplicity of different boundary conditions, such as different combinations of "open" and "closed" boundary conditions for reactor inlets and exits or for semiinfinite or infinite regions, and corresponding solutions occupy much of the literature over the past forty years (see Nauman, 1981 and Kreft and Zuber, 1978). For some relatively simple problems the analytical solutions have not even been available until now (see Kreft and Zuber, 1978). Application of the wave model permits us to avoid the uncertainties in the boundary conditions and thereby essentially to reduce the number of possible variants of solutions.

The wave model also has a wider region of validity. It is able to describe phenomena that cannot be explained in terms of the SDM. Dispersion during flow reversal and the difference between apparent diffusivity for pulse propagation and backmixing under stationary conditions are examples of these phenomena. In addition, the wave model gives a qualitatively correct concentration distribution for arbitrary time moments for pulse propagations through a system; it also gives exact long-time asymptotic values of the first three spatial moments of concentration for the case of Taylor dispersion and qualitatively correct steady-state concentration distributions for arbitrary chemical reaction rates.

Physical meaning and experimental determination of the model parameters

Model parameters have a clear physical sense. The dispersion coefficient D_e has the same sense as in the SDM: it characterizes the dispersion flux or the increase of the variance when the concentration distribution is close to equilibrium. The relaxation time τ can be considered to be a characteristic time, corresponding to the time of the mean free path of the diffusion process. After Taylor (1953) for Taylor dispersion phenomena, the relaxation time is also known as the "time of decay" during which transverse variations of concentration are reduced to a fraction of their initial value through the action of transverse dispersion. For laminar flow through a tube of a radius a, the relaxation time is $\tau = a^2/(15\ D)$, and the estimate of this time constant as $a^2/(3.8^2\ D)$ by Taylor (1953) is very close to the one obtained in this work. The relaxation time characterizes the inertia of the dispersion process or the rate of approaching equilibrium. The asymmetry parameter u_a characterizes the asymmetry of the dispersion process (see Eq. 30); it is determined by the differences in the positive and negative convective velocity profiles in a coordinate system moving with average velocity, and it is equal to the difference in the absolute values of the wave velocities in such a coordinate system. The importance of the model parameters for a quantitative treatment of chemical reactor problems will be considered in a subsequent article.

The wave model permits simple analytical solutions for various linear problems. Some of them are presented in this work. The solutions can be used for determination of the parameters of the model. The model parameters can be obtained by the standard experimental methods, which are used for the determination of longitudinal dispersion coefficients, in particular by the method of moments or the frequency response technique. The parameters of the model can be calculated by comparing the time moments of responses measured at two or more points along an apparatus or two or more spatial moments. Equations 23 to 25, 32, and 33 and their asymptotic forms obtained show that the model parameters can be obtained through knowledge of the long-term and short-term behavior of the first and second axial or time moments of the solute concentration fields. Two experimental studies—the change with time of the variance of a concentration pulse when the flow direction is reversed, and the difference in values of the apparent axial dispersion coefficient and the backmixing coefficient in a system with real backmixing—show how conveniently this new method of the wave model gives new possibilities for determining model parameters (see, e.g., Eqs. 46 to 49).

Additional remarks on the wave model

The preceding analysis shows that for slowly varying concentration fields the wave model can be approximated by the SDM. The use of the wave model instead of the Fickian dispersion model, however, is justified in all circumstances including slow processes, even if the parameters τ and u_a of the wave model are unknown. If somebody has some difficulties with the calculation or experimental determination of these parameters, he may put $u_a = 0$ and τ equal to the characteristic time scale that determines the applicability of the SDM. This recommendation permits the avoidance of physical contradictions, the resolution of the problem of boundary conditions of the SDM, the acquisition of correct results for slow processes where the SDM is applicable, and the acquisition of an approximate description of fast processes where the Fickian model gives absolutely incorrect results.

Conclusion

The preceding results provide support for the theory developed by the authors and demonstrate the importance of accounting for relaxation effects in longitudinal mixing in chemical reactors and contactors. Evidently, the wave model is physically more realistic than the conventional Fickian-type model. It has a much wider region of validity, and in most cases, is also more preferable from the mathematical point of view.

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Notation

A = cross-sectional area of the flow
C = dimensionless area-averaged concentration, c/c_{ch}
J = dimensionless dispersion flux, $j/(uc_{ch})$
L = reactor length
$m = M/A$
$p = 2(u_1 - u)(u - u_2)u/(u_1 - u_2)^3$
P = dimensionless parameter, t_{ch}/τ
q' = derivative of the consumption rate over concentration, $\partial q/\partial c$
Q = dimensionless consumption rate of component per unit of reactor volume, qt_{ch}/c_{ch}
$\bar{t}$ = mean residence time, Eq. 32
$u_{1,2}$ = characteristic or wave velocities in Eqs. 1 and 2, $u + (u_a/2)[1 \pm \sqrt{1 + 4D_e/(\tau u_a^2)}\,]$
u_a = parameter of velocity asymmetry
u_a^* = dimensionless parameter of velocity asymmetry, u_a/u
X = dimensionless longitudinal coordinate, $x/(ut_{ch})$
$Y = 2(\beta_1 \beta_2 \eta_1 \eta_2)^{1/2}$

Greek letters

β_i = parameter ($i = 1, 2$), Eq. 18
η_i = dimensionless variable ($i = 1, 2$), Eq. 18
θ = dimensionless time, t/t_{ch}
Λ = dimensionless value of the inlet concentration gradient, Eq. 7
μ_n = central spatial moment ($n = 2, 3, \ldots$), Eq. 21

Subscripts

1, 2 = before and after reversal of the flow
0 = inlet at $x = 0$ in the entering stream

Literature Cited

Aris, R., "On the Dispersion of Solute in a Fluid Flowing Through a Tube," *Proc. Roy. Soc. London*, **235A**, 67 (1956).

Aris, R., and N. R. Amundson, *Mathematical Methods in Chemical Engineering*, Vol. 2. *First-Order Partial Differential Equations with Applications*, Prentice-Hall, Englewood Cliffs, NJ (1973).

Barton, N. G., "Solute Dispersion and Weak Second-Order Recombination at Large Times in Parallel Flow," *J. Fluid Mech.*, **164**, 289 (1986).

Brenner, H., "A General Theory of Taylor Dispersion Phenomena," *Physicochem. Hydrody.*, **1**, 91 (1980).

Brenner, H., "A General Theory of Taylor Dispersion Phenomena: II. An Extension," *Physicochem. Hydrody.*, **3**, 139 (1982).

Brenner, H., and D. A. Edwards, *Macrotransport Processes*, Butterworth-Heinemann, Boston, 1993.

Chatwin, P. C., "The Approach to Normality of the Concentration Distribution of a Solvent Flowing Along a Straight Pipe," *J. Fluid Mech.*, Part 2, **43**, 321 (1970).

Fischer, H. B., E. J. List, R. C. Y. Koh, J. Imberger, and N. H. Brooks, *Mixing in Inland and Coastal Waters*, Academic Press, New York (1979).

Hiby, J. W., "Longitudinal and Transverse Mixing During Single-Phase Flow Through Granular Beds," in *Proc. Symp. on the Interaction Between Fluids and Particles*, The Institution of Chemical Engineers, London, p. 312 (1962).

Jasti, J. K., and H. S. Fogler, "Application of Neutron Radiography to Image Flow Phenomena in Porous Media," *AIChE J.*, **38**, 481 (1992).

Korenaga, T., F. Shen, and T. Takahashi, "An Experimental Study of the Dispersion in Laminar Tube Flow," *AIChE J.*, **35**, 1395 (1989).

Kreft, A., and A. Zuber, "On the Physical Meaning of the Dispersion Equation and its Solutions for Different Initial and Boundary Conditions," *Chem. Eng. Sci.*, **33**, 1471 (1981).

Maron, V. I., "Longitudinal Diffusion in a Flow Through a Tube," *Int. J. Multiphase Flow*, **4**, 339 (1978).

Nauman, E. B., "Residence Time Distributions in Systems Governed by the Dispersion Equation," *Chem. Eng. Sci.*, **36**, 957 (1981).

Novy, R. A., H. T. Davis, and L. E. Scriven, "Upstream and Downstream Boundary Conditions for Continuous-Flow Systems," *Chem. Eng. Sci.*, **45**, 1515 (1990).

Smith, R., "A Delay-Diffusion Description for Contaminant Dispersion," *J. Fluid Mech.*, **105**, 469 (1981).

Stewart, W. E., "Transport Phenomena in Fixed-Bed Reactors," *AIChE Symp. Ser.*, **61**(58), 61 (1965).

Takahashi, T., T. Korenaga, and F. Shen, "A Numerical Solution for the Dispersion in Laminar Flow Through a Circular Tube," *Can. J. Chem. Eng.*, **68**, 191 (1990).

Taylor, G., "Diffusion by Continuous Movements," *Proc. London Math. Soc.*, ser. 2, **20**, 196 (1921).

Taylor, G., "Dispersion of Soluble Matter in Solvent Flowing Slowly Through a Tube," *Proc. R. Soc. London*, **A219**, 186 (1953).

Tikhonov, A. N., and A. A. Samarskii, *Equations of Mathematical Physics*, Pergamon, Oxford (1963).

Thacker, W. C., "A Solvable Model of Shear Dispersion," *J. Phys. Oceanog.*, **6**, 66 (1976).

Wang, J. C., and W. E. Stewart, "New Description of Dispersion in Flow Through Tubes: Convolution and Collocation Methods," *AIChE J.*, **29**, 493 (1983).

Wang, J. C., and W. E. Stewart, "Multicomponent Reactive Dispersion in Tubes: Collocation vs. Radial Averaging," *AIChE J.*, **35**, 490 (1989).

Westerterp, K. R., V. V. Dil'man, and A. E. Kronberg, "The Wave Model for Longitudinal Dispersion: Development of the Model," *AIChE J.*, **41**, 2013 (1995).

Westerterp, K. R., and P. Landsman, "Axial Mixing in a Rotating Disk Contactor: I. Apparent Longitudinal Diffusion," *Chem. Eng. Sci.*, **17**, 363 (1962).

Westerterp, K. R., and W. H. Meyberg, "Axial Mixing in a Rotating Disk Contactor: II. Backmixing," *Chem. Eng. Sci.*, **17**, 373 (1962).

Westerterp, K. R., W. P. M. Van Swaaij, and A. A. C. M. Beenackers, *Chemical Reactor Design and Operation*, Wiley, Chichester, England (1987).

Whitham, G. B., *Linear and Nonlinear Waves*, Wiley-Interscience, New York (1974).

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