

Taylor limit of equilibration and the multimode diffusion approximation

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Abstract. The multimode diffusion approximation for solute dispersion in transversely bounded shear flows owes its origin to the formal method of eigenmode expansion. It is put forth upon the premise that a quasi-steady condition termed the Taylor limit of equilibrium exists in the course of time when equilibrium estimates of the residual terms of the concentration distribution can be realistically made contingent to the evolution of their primary counterparts. By applying the Green's function for the diffusion equation, this paper provides a qualifying account for the establishment of the Taylor limit. A method of successive approximations is derived for the determination of the principal mode coefficient functions with the inclusion of bulk reaction and longitudinal diffusion. The resulting equations governing the evolution of these mode coefficient functions are truncated to conform to the multimode diffusion type and the special Taylor-limit results given by Smith are easily deduced. Examples are given to illustrate the attainment of a convergent solution.

1. Introduction

The effects of cross-stream diffusion and longitudinal velocity shear on the dispersion and transport of a solute in laterally bounded rectilinear flows have been investigated by many authors. Though the basic contributing physical principles are qualitatively easy to understand, the quantitative assessment of the time evolution of the solute concentration governed by the underlying convection-diffusion equation, however, has led to much complicated mathematics. It was first concluded by Taylor [1] for dispersion in flow through straight circular pipes that at sufficiently large times the area-weighted transverse average solute concentration satisfies, in a coordinate moving with the mean flow velocity, a diffusion equation having a constant coefficient. Aris [2] and Chatwin [3] subsequently proved Taylor's conclusion from their theoretical analyses of the rectilinear pipe flow dispersion problem. The asymptotic model of Taylor dispersion has been generalized to describe diffusive transport in flows prescribed by curvilinear coordinates (see for example Frankel and Brenner [4]). At the other extreme, Lighthill [5] has derived a solution applicable at small times for the very initial evolution of the solute concentration. Case-specific finite-difference solutions have been studied by Ananthkrishnan et al. [6] and Gill and Ananthkrishnan [7] using the explicit formulation, and by Akay [8] using a time-splitting method. The generalized dispersion theory advocated by Gill and Sankarasubramanian [9, 10], though targeted for the purpose of developing a solution that in principle can be applied at arbitrary times, is essentially limited to its second-order approximation for practical applications. This is because the explicit evaluation of the requisite higher-order phenomenological transport coefficients, which depend specifically on the imposed initial concentration distribution except when time becomes very large, turns out to be formidably difficult even for the simplest cases. The conditions under which this particular theory is valid

has only recently been established in general terms and it has been shown that for an inert solute the second-order dispersion approximation is only applicable asymptotically at large and small times after solute release [11]. Such an approximation, for an initial solute input with a concentration distribution symmetric about the moving origin, invariably yields a Gaussian distribution for the transverse average concentration which is known to be at variance with experimental evidence except when sufficient time has elapsed. In an attempt to remove the shortcomings of the dispersion approximation, Smith [12] has introduced a memory displacement theory which, in the course of simplification, is reduced to the delay-diffusion description for the determination of the area-weighted mean concentration. It has now been shown, however, that such a theory is unsatisfactory in its original proposed form except possibly perhaps under highly restricted conditions because what it represents is the lowest order approximation of a general formulation which is valid on the same basis as that of the generalized dispersion theory [11].

More recently, also by Smith [13], a method of multi-mode diffusion approximation has been formulated by recognizing the existence of a quasi-equilibrium condition, which is called the Taylor limit of equilibration, of the evolution process beyond some characteristic time which becomes smaller and smaller as the number of employed eigenmodes increases. By design, the local concentration in this method is considered to consist of a principal part, which is to be resolved from the evolution equations, and a residual part, which in the Taylor limit is prescribed to follow a gradient formula. The basis for using the latter prescription is justified from the observation that, for dispersion without bulk solute removal, the single mode calculation yields precisely the classical large time result of Taylor's. In this paper, the condition under which the Taylor limit of equilibration exists is examined and the multimode diffusion formulation is extended to include the use of the method of successive approximations.

After this work has been completed, the authors are brought to attention by the referee to the recent articles by Mercer and Roberts [14] and by Young and Jones [15] dealing with the generalized Taylor model of shear dispersion formulated on the basis of the center manifold theorem. The theory correctly predicts the centroid, variance, and the higher moments of the transverse mean concentration distribution asymptotically at large times when the dispersion coefficients have all essentially reached their steady-state values. The multimode diffusion approximation to be dealt with in this paper, however, can be applied at arbitrary times, including the period of preasymptotic dispersion which is not accessible by the center manifold description.

2. Dispersion of solute with bulk depletion and boundary absorption

In keeping with the generality of the dispersion concept, we shall be concerned in this paper with the dispersion of a solute in the course of time subsequent to its release into a laterally bounded rectilinear flow field by including first-order bulk depletion and boundary absorption. The local solute concentration $c(x, y, z, t)$, as a function of the longitudinal distance x , the transverse location (y, z) , and time t , satisfies the full equation of convective diffusion

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2} + \nabla \cdot (\kappa_i \nabla c) - u \frac{\partial c}{\partial x} - k_A c + q \delta(t) \quad (1a)$$

together with the boundary condition

$$\kappa_i \mathbf{n} \cdot \nabla c + k_s c = 0 \quad \text{on } \partial A . \quad (1b)$$

Here ∇ is the transverse gradient operator, \mathbf{n} the outward normal to the transverse boundary ∂A , $q(x, y, z)$ the instantaneous initial rate of solute injection, $\delta(t)$ the Dirac delta function and, for the purpose of generality, we shall allow the coefficients in the above equations to vary over the transverse cross-section in the analysis. Thus, $\kappa(y, z)$ is the longitudinal diffusivity, $\kappa_i(y, z)$ the transverse diffusivity, $u(y, z)$ the longitudinally rectilinear flow velocity, and $k_A(y, z)$ and $k_s(y, z)$ are the reaction rate coefficients for bulk depletion and boundary absorption, respectively.

The eigenmode problem of transverse diffusion prescribed by the set of equations

$$\left. \begin{aligned} \nabla \cdot (\kappa_i \nabla \psi_j) &= \lambda_j \psi_j = 0 , \\ \kappa_i \mathbf{n} \cdot \nabla \psi_j + k_s \psi_j &= 0 \quad \text{on } \partial A , \end{aligned} \right\} \quad (2)$$

generates an infinite set of orthonormal eigenfunctions $\psi_j(y, z)$ corresponding to the eigenvalues λ_j which are non-negative, discrete, and denumerably countable without limit because of the boundedness of the lateral region by definition. Thus, we specify

$$\overline{\psi_j \psi_k} = \delta_{jk} , \quad (3)$$

$$0 \leq \lambda_0 < \lambda_1 < \lambda_2 < \dots , \quad (4)$$

where δ_{jk} is the Kronecker delta and an overbar is used to indicate averaging over the transverse cross-sectional area.

It is convenient and also appropriate to prescribe in principle a representation of the solute concentration in the form of the series expansion [16]

$$c(x, y, z, t) = \sum_{j=0}^{\infty} c_j(x, t) \psi_j(y, z) . \quad (5)$$

With this solution substituted into equation (1a), multiplying the result by ψ_j (j fixed), and then integrating over the transverse flow cross-section, we obtain the exact equations governing the evolution of the longitudinal coefficient functions $c_j(x, t)$

$$\frac{\partial c_j}{\partial t} + \sum_{k=0}^{\infty} \left(\beta_{jk} c_k + u_{jk} \frac{\partial c_k}{\partial x} - \kappa_{jk} \frac{\partial^2 c_k}{\partial x^2} \right) = q_j \delta(t) , \quad \text{for } j = 0, 1, \dots , \quad (6)$$

where the constant coefficients generated by eigenmode coupling for bulk depletion, convective transport, and longitudinal diffusion, respectively, are

$$\left. \begin{aligned} \beta_{jk} &= \lambda_j \delta_{jk} + \overline{k_A \psi_j \psi_k} , \\ 0 &\leq \beta_{00} < \beta_{11} < \dots , \end{aligned} \right\} \quad (7)$$

$$u_{jk} = \overline{u \psi_j \psi_k} , \quad (8)$$

$$\kappa_{jk} = \overline{\kappa \psi_j \psi_k} , \quad (9)$$

and the strength of the eigenmode forcing term due to the initial solute release is

$$q_j(x) = \overline{q(x, y, z)\psi_j(y, z)}. \quad (10)$$

3. Residual functions and multimode approximations

To facilitate formulating the method of multimode approximation, the local solute concentration is written in the form

$$c(x, y, z, t) = \sum_{j=0}^{N-1} c_j \psi_j + \sum_{n=N}^{\infty} c_n \psi_n, \quad (11)$$

where the first sum is the principal part to be functionally resolved with the use of an estimate of the second sum, which is called the residual part, under the condition of the Taylor limit of equilibration. We write the governing equations of the principal and residual longitudinal coefficient functions in the following forms which seem particularly suited for the multimode description

$$\frac{\partial c_j}{\partial t} + \sum_{k=0}^{N-1} \left(\beta_{jk} c_k + u_{jk} \frac{\partial c_k}{\partial x} - \kappa_{jk} \frac{\partial^2 c_k}{\partial x^2} \right) + \sum_{n=N}^{\infty} \left(\beta_{jn} c_n + u_{jn} \frac{\partial c_n}{\partial x} - \kappa_{jn} \frac{\partial^2 c_n}{\partial x^2} \right) = q_j \delta(t),$$

for $j = 0, 1, \dots, N-1$. (12)

$$\begin{aligned} \frac{\partial c_n}{\partial t} + \beta_{nn} c_n + u_{nn} \frac{\partial c_n}{\partial x} - \kappa_{nn} \frac{\partial^2 c_n}{\partial x^2} = & - \sum_{k=0}^{N-1} \left(\beta_{nk} c_k + u_{nk} \frac{\partial c_k}{\partial x} - \kappa_{nk} \frac{\partial^2 c_k}{\partial x^2} \right) + q_n \delta(t) \\ & - \sum_{m=N}^{\infty} (1 - \delta_{nm}) \left(\beta_{nm} c_m + u_{nm} \frac{\partial c_m}{\partial x} - \kappa_{nm} \frac{\partial^2 c_m}{\partial x^2} \right) \end{aligned}$$

for $n \geq N$. (13)

In what follows we present in a cookbook fashion the formulation of the first few low-order schemes of approximation.

3.1. Baseline truncation

We shall assume that the series given by equation (5) converges uniformly to the mathematically rigorous solution satisfying the underlying convective diffusion equation. It then becomes possible, at the baseline level or the zeroth order approximation, to use the partial series, by including a sufficiently large number of modes N ,

$$c(x, y, z, t) \approx \sum_{j=0}^{N-1} c_j(x, t) \psi_j(y, z), \quad (14)$$

as an approximate representation of the solute concentration. This approximation is valid at times when the residual functions are negligibly small and therefore any contributions arising from these terms in equation (12) can be discarded, and correspondingly one has the approximate evolution equations

$$\frac{\partial c_j}{\partial t} + \sum_{k=0}^{N-1} \left(\beta_{jk} c_k + u_{jk} \frac{\partial c_k}{\partial x} - \kappa_{jk} \frac{\partial^2 c_k}{\partial x^2} \right) = q_j \delta(t), \quad \text{for } j=0, 1, \dots, N-1. \quad (15)$$

Equation (15) defines a set of N linear equations with constant coefficients for the determination of the principal mode coefficient functions c_j ($j \leq N-1$). These equations, which can be solved by a host of routine techniques, are obviously useful for numerical computations with the use of a digital computer in the sense of convergence in the mean. For an efficient representation, the number of terms of the series N must be large enough so that little or no contributions to $c(x, y, z, t)$ arise from the eigenmodes of orders equal to and higher than N . For systematic determination of the convergent solution in practice, a suitable convergence criterion serving to check the efficiency of the representation must therefore be provided in the computation process after each step the number of terms N is incremented.

3.2. First order approximation

A somewhat more efficient description can be formulated by making use of equation (13) which serves to estimate the residual mode coefficient functions. As a first approximation, again by making the number of principal modes N sufficiently large, the second summation term in equation (13) can be neglected and we have the approximate governing equations

$$\frac{\partial c_n}{\partial t} + \beta_{nn} c_n + u_{nn} \frac{\partial c_n}{\partial x} - \kappa_{nn} \frac{\partial^2 c_n}{\partial x^2} = - \sum_{k=0}^{N-1} \left(\beta_{nk} c_k + u_{nk} \frac{\partial c_k}{\partial x} - \kappa_{nk} \frac{\partial^2 c_k}{\partial x^2} \right) + q_n \delta(t), \quad n \geq N. \quad (16)$$

Consequently the residual longitudinal coefficient functions become deterministic in terms of their principal counterparts.

In the above equation, the diffusivity κ_{nn} and the bulk rate coefficient β_{nn} associated with eigenmode ψ_n are constant and the summation term can be regarded as a continuous source because it is independent of the particular function c_n which the present equation seeks to determine under the imposed conditions that $c_n \rightarrow 0$ as $x \rightarrow \pm\infty$. The solution is

$$c_n(x, t) = \rho_n(x, t) - \sum_{k=0}^{N-1} \int_0^t dt_s \int_{-\infty}^{\infty} dx_s \left(\beta_{nk} c_k + u_{nk} \frac{\partial c_k}{\partial x_s} - \kappa_{nk} \frac{\partial^2 c_k}{\partial x_s^2} \right) G_n(x, t | x_s, t_s) \quad (17)$$

for $n \geq N$,

where

$$G_n(x, t | x_s, t_s) = \frac{1}{2\sqrt{\pi\kappa_{nn}(t-t_s)}} \exp\left\{ -\frac{[x-x_s-u_{nn}(t-t_s)]^2}{4\kappa_{nn}(t-t_s)} - \beta_{nn}(t-t_s) \right\}, \quad (18)$$

is the Green's function for diffusion generated by an instantaneous point source of strength unity released at time t_s and location x_s in the source coordinates (see for example Morse and Feshback [17]), and

$$\rho_n(x, t) = \frac{1}{2\sqrt{\pi\kappa_{nn}t}} e^{-\beta_{nn}t} \int_{-\infty}^{\infty} q_n(x_s) \exp\left[-\frac{(x-u_{nn}t-x_s)^2}{4\kappa_{nn}t} \right] dx_s \quad (19)$$

is the contribution to c_n arising from the initial distribution exclusively due to longitudinal diffusion, i.e., as if lateral diffusion were completely absent.

It can readily be inferred from the integral solution of equation (17) that, because the Green's function of equation (18) decays exponentially in time according to $\exp[-\beta_{nn}(t - t_s)]$, the evolving of the eigenmode coefficient functions c_n depends critically on the events occurred immediately prior to the present time t within a characteristic time duration of the order of $1/\beta_{nn}$. The diagonal coefficients β_{nn} , as has been specified in equation (7), are non-negative and form an ascending sequence. As the number of principal modes N included in the approximation of equation (16) increases, the exponential time decays of the residual functions therefore become progressively more rapid, and correspondingly the characteristic time durations decrease indefinitely toward zero. It then follows that if the mode number N is sufficiently large and the effective time interval consequently becomes sufficiently small, the Green's function contributing to the integral of equation (17) will become so sharply peaked that, by using the limiting representations,

$$\beta_{nn} \exp[-\beta_{nn}(t - t_s)] = \delta(t - t_s), \quad \beta_{nn} \rightarrow \infty, \quad (20)$$

and

$$\frac{1}{2\sqrt{\pi\kappa_{nn}\Delta t}} \exp\left[-\frac{(x - x_s - u_{nn}\Delta t)^2}{4\kappa_{nn}\Delta t}\right] = \delta(x - x_s), \quad \Delta t \rightarrow 0, \quad (21)$$

we are qualified to write, for sufficiently large β_{nn} ,

$$G_n(x, t | x_s, t_s) \rightarrow \frac{1}{\beta_{nn}} \delta(x - x_s) \delta(t - t_s), \quad \beta_{nn} \rightarrow \infty, \quad (22)$$

where $\delta(x)$ is the Dirac delta function. Also at times such that,

$$\beta_{NNt} \gg 1, \quad (23)$$

the residual mode coefficient functions c_n associated with the higher modes ψ_n have essentially lost their memories about their initial identities because the functions $\rho_n(x, t)$ of equation (19), on account of $\beta_{nn} \gg \beta_{NN}$, effectively have all decayed to zero.

Use of the above limiting form of the Green's function in equation (17) while imposing the condition of equation (23) leads us to the asymptotic expression

$$c_n(x, t) = -\frac{1}{\beta_{nn}} \sum_{k=0}^{N-1} \left(\beta_{nk} c_k + u_{nk} \frac{\partial c_k}{\partial x} - \kappa_{nk} \frac{\partial^2 c_k}{\partial x^2} \right) \quad \text{for } n \geq N, \quad (24)$$

which clearly is a version of the multimode approximation when bulk depletion, convective transport, and longitudinal diffusion are all taken into account. It is thus seen, as is also the case with Smith, that under the Taylor limit of equilibration which presently can be defined as a condition at times after solute release so that the qualification requirements of equations (22) and (23) are reasonably met, the residual terms become quasi-steady in character by being concomitant to the principal terms in origin. It is to be noted, however, that, at a time required by the condition of equation (23), this is valid only if a large number of modes are included in the approximation, i.e., if the limiting form of the Green's function becomes tolerably meaningful.

If the asymptotic expression of equation (24) is used in equation (12) and x -derivatives only up to the second order are retained after the substitution, we obtain the following set of coupled equations serving to resolve approximately the N principal mode coefficient functions

$$\frac{\partial c_i}{\partial t} + \sum_{k=0}^{N-1} \left(B_{jk} c_k + U_{jk} \frac{\partial c_k}{\partial x} - K_{jk} \frac{\partial^2 c_k}{\partial x^2} \right) = q_j(x) \delta(t),$$

$$\beta_{NN} t \gg 1, \quad j = 0, 1, \dots, N-1,$$
(25)

where

$$B_{jk} = \beta_{jk} - \sum_{n=N}^{\infty} \frac{\beta_{jn} \beta_{nk}}{\beta_{nn}}, \quad U_{jk} = u_{jk} - \sum_{n=N}^{\infty} \frac{\beta_{jn} u_{nk} + u_{jn} \beta_{nk}}{\beta_{nn}},$$

$$K_{jk} = \kappa_{jk} + \sum_{n=N}^{\infty} \frac{u_{jn} u_{nk} - \beta_{jn} \kappa_{nk} - \kappa_{jn} \beta_{nk}}{\beta_{nn}}.$$
(26)

At long enough times, the solute spreads out longitudinally over a large distance so that we can use the above diffusion approximation by neglecting the x -derivatives of orders 3 and higher.

3.3. Higher order approximations

To obtain the next higher level of approximation for perhaps a somewhat closer estimate of the residual coefficient functions, the first-order expression of equation (24) for c_n is used in the second sum of equation (13) to yield

$$\frac{\partial c_n}{\partial t} + \beta_{nn} c_n + u_{nn} \frac{\partial c_n}{\partial x} - \kappa_{nn} \frac{\partial^2 c_n}{\partial x^2} = - \sum_{k=0}^{N-1} \left(\beta'_{nk} c_k + u'_{nk} \frac{\partial c_k}{\partial x} - \kappa'_{nk} \frac{\partial^2 c_k}{\partial x^2} \right) + q_k \delta(t), \quad n \geq N,$$
(27)

where again, within the limit of diffusion approximation, x -derivatives of orders 3 and higher have been ignored, and the mode coupling coefficients are given by

$$\beta'_{nk} = \beta_{nk} - \sum_{m=N}^{\infty} (1 - \delta_{nm}) \frac{\beta_{nm} \beta_{mk}}{\beta_{mm}}, \quad u'_{nk} = u_{nk} - \sum_{m=N}^{\infty} (1 - \delta_{nm}) \frac{\beta_{nm} u_{mk} + u_{nm} \beta_{mk}}{\beta_{mm}},$$

$$\kappa'_{nk} = \kappa_{nk} + \sum_{m=N}^{\infty} (1 - \delta_{nm}) \frac{u_{nm} u_{mk} - \beta_{nm} \kappa_{mk} - \kappa_{nm} \beta_{mk}}{\beta_{mm}}.$$
(28)

Thus, if a sufficiently large number of principal modes N is included in the calculation so that the limiting form of the Green's function given by equation (22) for establishing the Taylor limit of equilibration applies, we then have for the residual coefficient functions,

$$c_n(x, t) = - \frac{1}{\beta_{nn}} \sum_{k=0}^{N-1} \left(\beta'_{nk} c_k + u'_{nk} \frac{\partial c_k}{\partial x} - \kappa'_{nk} \frac{\partial^2 c_k}{\partial x^2} \right) \quad \text{for } n \geq N,$$
(29)

which can now be used in equation (12) to yield the diffusion equations for resolving the principal coefficient functions in the second-order approximation,

$$\frac{\partial c_j}{\partial t} + \sum_{k=0}^{N-1} \left(B'_{jk} c_k + U'_{jk} \frac{\partial c_k}{\partial x} - K'_{jk} \frac{\partial^2 c_k}{\partial x^2} \right) = q_j(x) \delta(t),$$

$$\beta_{NN} t \gg 1, \quad j = 0, 1, \dots, N-1,$$
(30)

where

$$B'_{jk} = \beta_{jk} - \sum_{n=N}^{\infty} \frac{\beta_{jn} \beta'_{nk}}{\beta_{nn}}, \quad U'_{jk} = u_{jk} - \sum_{n=N}^{\infty} \frac{\beta_{jn} u'_{nk} + u_{jn} \beta'_{nk}}{\beta_{nn}},$$

$$K'_{jk} = \kappa_{jk} + \sum_{n=N}^{\infty} \frac{u_{jn} u'_{nk} - \beta_{jn} \kappa'_{nk} - \kappa_{jn} \beta'_{nk}}{\beta_{nn}}.$$
(31)

Equation (29) can now be used in equation (13) to obtain the third-order multimode formulation. The extension to higher orders by successive approximations is obvious.

4. Results of Smith for dispersion with constant bulk reaction rate

The extended Taylor limit suggested by Smith [13] for flows with constant bulk reaction rate coefficients k_A (specifically Smith considered $k_A = 0$) can be obtained in a rather trivial manner from the above asymptotic approximations. Under such stipulations one has from equations (7)

$$\beta_{jk} = (\lambda_j + k_A) \delta_{jk}.$$
(32)

It then suffices that we use a gradient formula equivalent to that of Smith who provided its derivation by making equilibrium estimates of the residual parts through a delicate procedure using time-decaying temporary expedients,

$$c_k(x, t) = -\frac{1}{\lambda_k + k_A} \sum_{n=0}^{N-1} u_{kn} \frac{\partial c_n}{\partial x} \quad \text{for } k \geq N,$$
(33)

which presently can be obtained from either equation (24) or equation (29) by discarding the term containing $\partial^2 c_k / \partial x^2$ as a factor because it contributes nothing to the evolution of the principal coefficient functions in the form of either equation (25) or equation (30). It thus follows that

$$B'_{jk} = B_{jk} = (\lambda_j + k_A) \delta_{jk}, \quad U'_{jk} = U_{jk} = u_{jk}, \quad K'_{jk} = K_{jk} = \kappa_{jk} + \sum_{n=N}^{\infty} \frac{u_{jn} u_{nk}}{\lambda_n + k_A},$$
(34)

and we arrive at the equations pertaining to the multimode diffusion approximation

$$\frac{\partial c_j}{\partial t} + (\lambda_j + k_A) c_j + \sum_{k=0}^{N-1} u_{jk} \frac{\partial c_k}{\partial x} - \sum_{k=0}^{N-1} (\kappa_{jk} + D_{jk}) \frac{\partial^2 c_k}{\partial x^2} = q_j(x) \delta(t), \quad j = 0, 1, \dots, N-1,$$
(35)

where the dispersion coefficient purely arising from the velocity shear is given by

$$D_{jk} = \sum_{n=N}^{\infty} \frac{u_{jn}u_{nk}}{\lambda_n + k_A}. \quad (36)$$

The shear dispersion coefficients given by Smith have the same expression as above with $k_A = 0$ except that $\lambda_n - \lambda_k$ appears there in the denominator. The difference is of little or no consequence, however, because both formulations will eventually converge to the same solutions if enough principal modes are used in the approximation.

5. Dispersion of an inert solute in laminar pipe flow

To apply the multimode approximations for illustrating the attainment of a convergent solution, we consider here, using the initial-value problem originally posed by Taylor [1], the dispersive transport of an inert solute ($k_A = 0$) in laminar pipe flow with a constant and isotropic diffusivity ($\kappa = \kappa_i$) for the determination of the area-weighted transverse average concentration. The needed recipes for this case are given by equation (15) for the baseline truncation scheme and equation (35) for the higher order multimode approximations.

The pipe wall, having a radius a , is nonabsorptive and impermeable ($k_s = 0$) so that

$$\partial c / \partial r = 0 \quad \text{at } r = a; \quad (37)$$

the flow is laminar with a velocity profile

$$u = u_0(1 - r^2/a^2), \quad (38)$$

with u_0 being the centerline velocity, and the source strength due to the initial solute release is radially uniform, i.e., $q(x, r) = q(x)$ which is a square-integrable function of the axial coordinate x , meaning that the solute in the pipe is finite in total amount.

The essential characteristic quantities of this particular problem are well known. The transverse eigenfunctions and eigenvalues are

$$\psi_j = \frac{J_0(\gamma_j r/a)}{a\sqrt{\pi}J_0(\gamma_j)}, \quad \lambda_j = \frac{\gamma_j^2 \kappa}{a^2}, \quad \text{with } J_1(\gamma_j) = 0 \quad \text{for } j = 0, 1, 2, \dots, \quad (39)$$

where γ_j is an increasing sequence starting with $\gamma_0 = 0$. Then the area-weighted transverse average concentration is

$$\bar{c}(x, t) = c_0(x, t), \quad (40)$$

the strength of eigenmode forcing arising from the initial source release is

$$q_j(x) = q(x)\delta_{j0}, \quad (41)$$

and the eigenmode-coupling velocities have the explicit expressions

$$u_{00} = \frac{1}{2} u_0; \quad u_{jj} = \frac{2}{3} u_0 \quad \text{for } j \geq 1; \quad \text{and } u_{jk} = -\frac{4(\gamma_j^2 + \gamma_k^2)}{(\gamma_j^2 - \gamma_k^2)^2} u_0 \quad \text{for } k \neq j. \quad (42)$$

The shear dispersion coefficients defined by (29) are then given by

$$D_{jk} = 16\kappa \text{Pe}^2 \sum_{n=N}^{\infty} \frac{(\gamma_n^2 + \gamma_j^2)(\gamma_n^2 + \gamma_k^2)}{\gamma_n^2(\gamma_n^2 - \gamma_j^2)^2(\gamma_n^2 - \gamma_k^2)^2}, \tag{43}$$

where we have introduced the diffusion Peclet number

$$\text{Pe} = au_0/\kappa. \tag{44}$$

The set of linear systems given by either equations (15) or (35) for the evolution of the principal coefficient functions c_j ($j = 0, 1, \dots, N - 1$) can be solved by applying the method of Laplace and Fourier transforms. In terms of the dimensionless variables

$$X = \frac{1}{a \text{Pe}} \left(x - \frac{u_0 t}{2} \right) \quad \text{and} \quad \tau = \frac{\kappa t}{a^2}, \tag{45}$$

it can be readily be shown that the area-weighted transverse average concentration has the approximate representation

$$\bar{c} = c_0 = \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{N-1} \int_{-\infty}^{\infty} F(\omega) \frac{B_n}{A_n'} \exp[a_n \tau + i(b_n \tau + \omega X)] d\omega, \tag{46}$$

where $i = \sqrt{-1}$,

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} q(X) e^{-i\omega X} dX, \tag{47}$$

with $q(X) \equiv q(x)$; $p = a_n + ib_n$ are the zeros of a characteristic determinant, call it $|A|$, having an element in the $(j + 1)$ th row and $(k + 1)$ th column given by

$$a_{jk} = \left(p + \lambda_j^2 + \frac{\omega^2}{\text{Pe}^2} \right) \delta_{jk} + \omega^2 d_{jk} + i\omega \left(\frac{u_{jk}}{u_0} - \frac{1}{2} \delta_{jk} \right) \quad \text{for } j, k = 0, 1, 2, \dots, N - 1, \tag{48}$$

with

$$d_{jk} = \begin{cases} 0 & \text{for baseline truncation} \\ D_{jk}/\kappa \text{Pe}^2 & \text{for multimode diffusion;} \end{cases} \tag{49}$$

$A_n' = d|A|/dp$, and B_n is the cofactor of the first element a_{00} of determinant $|A|$, both evaluated at $p = a_n + ib_n$.

For graphical illustration, we make use of the slug stimulus example numerically studied in detail by Gill and Ananthakrishnan [7] where the initial release is of uniform strength unity, that is,

$$q(X) = q(x) = \begin{cases} 1 & \text{for } |x| < x_i/2, \\ 0 & \text{for } |x| > x_i/2, \end{cases} \tag{50}$$

with a slug length $x_i/a = 6$ and a Peclet number $\text{Pe} = 1000$.

The solutions determined with increasing number of principal modes at a dimensionless time $\tau = 0.1$ by the baseline truncation scheme and the higher-order multimode diffusion approximations are shown in Figs. 1 and 2, respectively. The convergent solutions given by the solid lines in these graphs are essentially the same for all practical purposes. Before

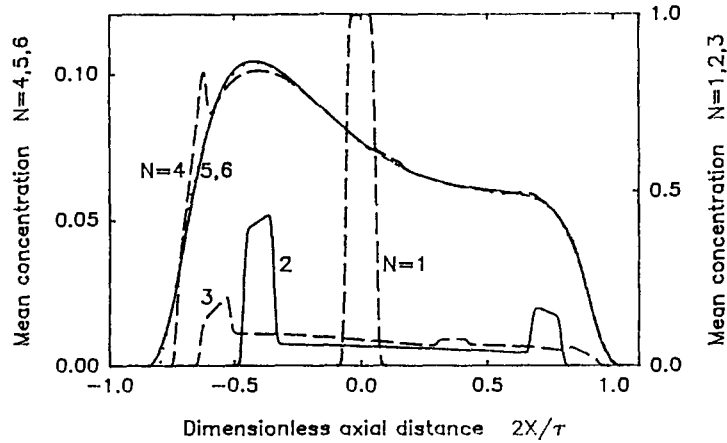


Fig. 1. Representations of the mean concentration distribution at $\tau = 0.1$ from the baseline truncation scheme with increasing mode number N . The solid line is good for $N \geq 6$.

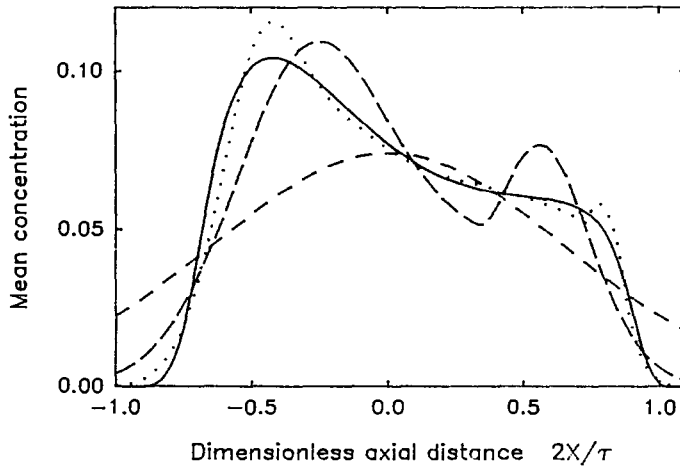


Fig. 2. Representations of the mean concentration distribution at $\tau = 0.1$ from higher order multimode approximations with mode numbers: $N = 1$ (---), $N = 2$ (—), $N = 3$ (····), $N \geq 5$ (-·-·-).

convergence is reached, it can be seen from these graphs that baseline truncations result in underestimating the effects due to the presence of the wall on the longitudinal dispersion of the solute. However, the multimode diffusion approximations for small N with the residual terms correlated by the limiting form of equation (22) for the Green's function turn out to do just the opposite by overestimating such longitudinal spread. The discrepancies are especially pronounced in the region far upstream of the distribution where the highest concentration occurs near the pipe wall and diffusion and convection are equally important in the local transport process of the solute. To obtain the common convergent solution (solid lines in both graphs), the number of principal modes required by multimode diffusion ($N \geq 5$) turns out to be one less than that by baseline truncation ($N \geq 6$), giving an edge to the former in computational efficiency.

The convergent solution at $\tau = 0.1$ is plotted in Fig. 3 together with the profiles

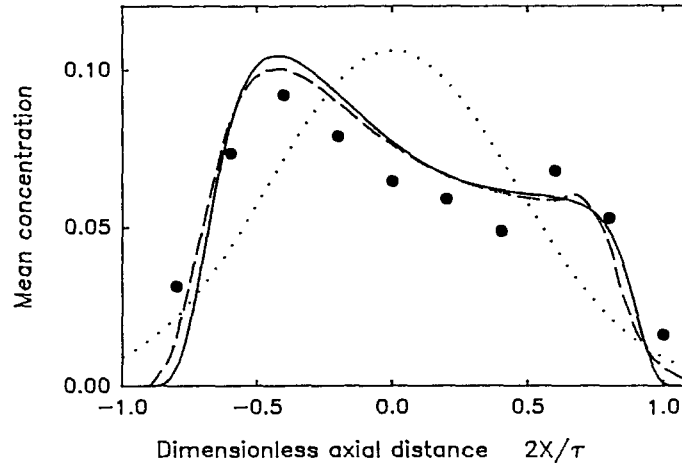


Fig. 3. Comparison of the mean concentration profiles at $\tau = 0.1$ given by different solutions: second-order dispersion of Gill and Sankarasubramanian [9] (\cdots), finite-difference of Gill and Ananthakrishnan [7] ($-\cdots-$), present ($—$), and delay-diffusion of Smith [12] ($\bullet\bullet\bullet$).

representing the transverse mean concentration distribution determined by other methods. The latter profiles were duplicated from the originally published graphs with an accuracy very close to three places. The presently calculated profile satisfies precisely the requirement of mass conservation and the condition that the centroid of the concentration distribution moves with the mean flow velocity [2]. It compares very well with the finite-difference result of Gill and Ananthakrishnan [7]. Neither the second-order dispersion approximation of Gill and Sankarasubramanian [10] nor the delay-diffusion prescription of Smith [13], however, enjoys such favorable comparison. Numerical computation of the present solution is a straightforward matter in obtaining both convergence and accuracy; solution of the convective diffusion equation by finite-difference formulation, on the other hand, has been found to necessitate a trial and error procedure in determining the increment sizes of the space and time variables solely for the purpose of achieving computational stability and solution convergence [6], perhaps with little or no possibility for the assessment of numerical accuracy. A close examination of the first moments of the finite-difference solution shows that the mass of the solute is conserved but the centroid of the distribution is somewhat at variance with the exact location moving with the mean flow velocity [2]. The slight but consistent discrepancy between these two solutions shown in Fig. 3 must therefore be attributed to the inaccuracy inherent from the use of the finite-difference scheme. As another numerical test, the convergent solutions at an earlier time $\tau = 0.05$ are compared in Fig. 4. Here the general patterns are about the same as those in the previous graph at $\tau = 0.1$ except the magnitude of the inaccuracy inherent of the finite-difference scheme becomes slightly worse. A comparison of the computed profiles at a typical large time of $\tau = 2.2$ is made in Fig. 5. It appears that the numerical results of Gill and Ananthakrishnan [7], though all three profiles agree reasonably well, seem to fare the worst in quantitative prediction, further illustrating the difficulty for achieving numerical accuracy associated with the use of the finite-difference scheme.

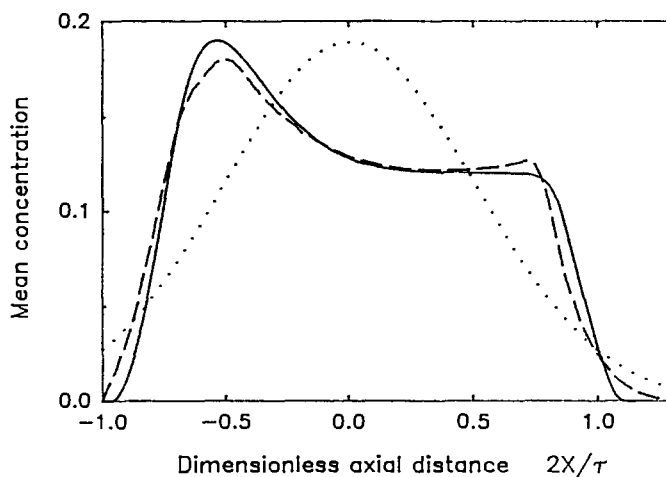


Fig. 4. Comparison of the mean concentration profiles at $\tau = 0.05$ given by different solutions: same captions as in Fig. 3.

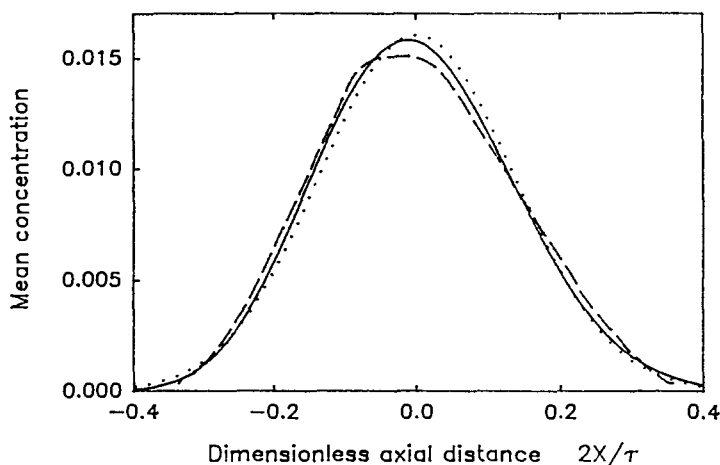


Fig. 5. Comparison of the mean concentration profiles at $\tau = 2.2$ given by different solutions: same captions as in Fig. 3.

6. Conclusions

The method of multimode diffusion approximation owes its origin in entirety to the formal method of eigenmode expansion for the local solute concentration. The condition under which the Taylor limit of equilibration exists, providing quasi-steady estimates for the residual mode coefficient functions of the concentration distribution in relation to their principal counterparts, is explored on a qualifying coherent basis through the use of the Green's function of diffusion. A method of successive approximations for the determination

of the principal mode coefficient functions is formulated. Unlike the center manifold description which is limited purely to asymptotic prediction, the multimode diffusion approximation can be applied to capture the preasymptotic dispersion behavior as well. For numerical evolution, the multimode formulation offers the distinctive advantage that the computation of the solution is steadfastly simple if the transverse eigenfunctions are known. In any case, the schemes are easy to use for dispersion in open or closed channel flows with simple transverse geometries.

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