New Descriptions of Dispersion in Flow Through Tubes: Convolution and Collocation Methods

The convective dispersion of a solute in steady flow through a tube is analyzed, and the concentration profile for any Peclet number is obtained as a convolution of the profile for infinite Peclet number. Close approximations are obtained for the concentration profile and its axial moments, by use of orthogonal collocation in the radial coordinate. The moments thus obtained converge rapidly, and the concentration profile less rapidly, toward exactness as the number of collocation points is increased. A two-point radial grid gives results of practical accuracy; analytical solutions are given at this order of approximation.

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SCOPE

Convective dispersion plays an important role in many processes of chemical reaction and separation. In process design, such systems are commonly analyzed by use of a radially-averaged diffusion equation. As a result of the averaging, the diffusion coefficient is replaced by an "axial dispersion coefficient" $\mathcal{D}_z$, determined from experiments or from prior analysis of a related problem. This time-honored approach gained credibility from the asymptotic analyses of Taylor (1953) and Aris (1956), which related the radially averaged description to a full two-dimensional one. Subsequent investigators (Lighthill, 1966; Gill and Sankarasubramanian, 1970, 1971, 1973; Chatwin, 1970, 1977; De Gance and Johns, 1978 a, b) have given more detailed solutions, also including radially-averaged values.

Radially-averaged equations have limited predictive power, since the dispersion coefficient is not a fluid property but a function determined by the given problem. For predictive purposes, either a direct scale-up technique or an efficient solution of the full diffusion equation should be preferred. In this paper we take the latter approach, and solve the full diffusion equation by orthogonal collocation in the radial direction. We demonstrate this approach for nonreactive systems here, and for reactive ones in a later paper.

CONCLUSIONS AND SIGNIFICANCE

The convolution relations in Eqs. 13 and 14 show clearly the influence of axial molecular diffusion on the performance of a pulsed transient system. The concentration profile at any Peclet number is obtained by Gaussian smoothing of the infinite-Pe solution. In the limit as $Pe \to \infty$ the diffusion is purely radial and neither species can travel upstream; thus, the back-diffusion which occurs at finite Peclet numbers is described entirely by the Gaussian smoothing.

The superposition solution in Eq. 38 shows the detailed influence of the initial condition on the concentration profile at any later time. This result, like the convolution in Eq. 14, reflects the linearity of the given problem.

Our main conclusion is that orthogonal collocation is a very good way to solve dispersion problems. Our comparisons with known exact solutions indicate that this method works well, down to very short diffusion times. The efficiency of the method is due to the simplicity of the radial profiles in the cases studied here, and also to the error-minimizing properties of the Gaussian quadrature points. Solutions with as few as two radial collocation points (for $n < 2$ no Taylor dispersion is predicted) are sufficiently accurate for many purposes. New boundary conditions and chemical kinetics are readily inserted, and nonlinear systems can be directly modelled.

INTRODUCTION

The collocation procedure described here is a variant of that given by Villadsen and Stewart (1967); see also Finlayson (1972) and Villadsen and Michelsen (1978). For axially symmetric states in a tubular reactor, we approximate the profile of each unknown state variable Y_m in the form

$$\tilde{Y}_m = \sum_{i=0}^{n} a_{im}(\tau,Z)\xi^{2i} \qquad 0 \leq \xi \leq 1. \tag{1}$$

This expansion can also be written as a Lagrange polynomial

$$\tilde{Y}_m = \sum_{k=1}^{n+1} W_k(\xi)\tilde{Y}_m(\tau,Z,\xi_k) \qquad 0 \leq \xi \leq 1 \tag{2}$$

with radial basis functions

$$W_k(\xi) = \prod_{j\neq k} (\xi^2 - \xi_j^2) \Big/ \prod_{j\neq k} (\xi_k^2 - \xi_j^2). \tag{3}$$

Thus, each approximate profile $\tilde{Y}_m$ is represented by Lagrange interpolation in terms of its values $\tilde{Y}_m(\tau,Z,\xi_k)$ at a set of chosen radial nodes ξ_k. We choose $\xi_1^2, \cdots \xi_n^2$ as the zeros of the shifted Legendre polynomial $P_n(x)$ (Abramowitz and Stegun, 1972) and add a node at the wall: $\xi_{n+1} = 1$.

Any needed derivatives or integrals of $\tilde{Y}_m$ can now be represented as linear combinations of the nodal values $\tilde{Y}_m(\xi_k)$; this is

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known as the method of ordinates (Villadsen and Stewart, 1967). For example, the dimensionless radial derivatives of interest at the radial node ξ_i are:

$$\left.\frac{d\tilde{Y}_m}{d\xi}\right|_{\tau,Z,\xi_i} = \sum_{k=1}^{n+1}\left[\left.\frac{d}{d\xi}W_k(\xi)\right|_{\xi_i}\right]\tilde{Y}_m(\tau,Z,\xi_k) = \sum_{k=1}^{n+1} A_{ik}\tilde{Y}_{mk}(\tau,Z) \quad (4)$$

$$\left.\frac{1}{\xi}\frac{d}{d\xi}\left(\xi\frac{d\tilde{Y}_m}{d\xi}\right)\right|_{\tau,Z,\xi_i} = \sum_{k=1}^{n+1}\left[\left.\frac{1}{\xi}\frac{d}{d\xi}\left(\xi\frac{dW_k}{d\xi}\right)\right|_{\xi_i}\right]\tilde{Y}_m(\tau,z,\xi_k) = \sum_{k=1}^{n+1} B_{ik}\tilde{Y}_{mk}(\tau,Z). \quad (5)$$

In this way, we reduce all radial derivatives to summations; the same can be done for differences and integrals with respect to ξ. For the above choice of nodes, weighted integrals of $\tilde{Y}_m$ over the cross-section can be obtained with high accuracy by use of Gauss' quadrature formula.

The boundary conditions at the wall may be linear or nonlinear. If they are linear, then $\tilde{Y}_{m,n+1}$ can be expressed linearly in terms of the interior values $\tilde{Y}_{mk}$ by use of the boundary condition and Eqs. 2 to 4. This permits elimination of $\tilde{Y}_{m,n+1}$ from Eq. 5; the resulting new weight coefficients in the one-component case will be denoted by B'_{ik}. Nonlinear boundary conditions, on the other hand, will generally require explicit inclusion of the boundary unknowns throughout the solution process.

CONVOLUTION RELATION

Consider the developed isothermal flow of a binary Newtonian or non-Newtonian fluid in an infinitely long circular tube. The density ρ and binary diffusivity $\mathcal{D}_{AB}$ are treated as constants. Chemical conversion of the solute, A, to the solvent, B, may occur at a rate locally linear in the solute concentration $\rho\omega$. The continuity equation for the solute may be written in the dimensionless form

$$\frac{\partial\omega}{\partial\tau} + V(\xi)\frac{\partial\omega}{\partial Z} = \frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\omega}{\partial\xi}\right) + \frac{1}{Pe^2}\frac{\partial^2\omega}{\partial Z^2} - K'''\omega \quad (6)$$

with the initial and boundary conditions

$$\text{At } \tau = 0\text{: } \omega(\tau,Z,\xi) = G(Z,\xi) \quad (7)$$

$$\text{At } \xi = 1\text{: } \frac{\partial}{\partial\xi}\omega(\tau,Z,\xi) + K''\omega(\tau,Z,\xi) = 0 \text{ for } \tau > 0 \quad (8)$$

$$\text{At } \xi = 0\text{: } \frac{\partial}{\partial\xi}\omega(\tau,Z,\xi) = 0 \text{ for } \tau > 0. \quad (9)$$

Here K''' and K'' are the first and second dimensionless numbers of Damköhler (1936) for homogeneous and heterogeneous reactions. Specific forms of the initial mass-fraction distribution $G(Z,\xi)$ will be considered presently. The Laplace-Fourier transform of Eqs. 6–9 from the domain of (τ,Z,ξ) into that of (s,p,ξ) is

$$\left(s + K''' - \frac{p^2}{Pe^2}\right)\bar{\bar{\omega}} + pV(\xi)\bar{\bar{\omega}} = \frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\bar{\bar{\omega}}}{\partial\xi}\right) + \bar{G}(p,\xi) \quad (10)$$

$$\text{At } \xi = 1\text{: } \frac{\partial}{\partial\xi}\bar{\bar{\omega}}(s,p,\xi) + K''\bar{\bar{\omega}}(s,p,\xi) = 0 \quad (11)$$

$$\text{At } \xi = 0\text{: } \frac{\partial}{\partial\xi}\bar{\bar{\omega}}(s,p,\xi) = 0. \quad (12)$$

Let ω_∞ be the solution of Eqs. 6–9 with longitudinal molecular diffusion neglected, i.e., with infinite Peclet number Pe. The transform $\bar{\bar{\omega}}_\infty$ of this solution satisfies Eqs. 10–12 with the p^2 term suppressed. Use of the s-shift theorem and Fourier convolution theorem (Campbell and Foster, 1967) then gives:

$$\bar{\omega}(\tau,p,\xi) = \exp\left(\frac{p^2\tau}{Pe^2}\right)\bar{\omega}_\infty(\tau,p,\xi) \quad (13)$$

$$\omega(\tau,Z,\xi) = \int_{-\infty}^{\infty}\frac{Pe}{2\sqrt{\pi\tau}}\exp\left[-\frac{Pe^2}{4\pi\tau}(Z - X)^2\right]\omega_\infty(\tau,X,\xi)dX. \quad (14)$$

Thus, the complete solution of Eqs. 6–9 is obtained by Gaussian smoothing of the infinite-Pe solution.

TWO-POINT COLLOCATION; NONREACTIVE CASE

Let C_∞ be the solution of Eqs. 6–9 with $K'' = K''' = 0$, $Pe = \infty$, and the following initial mass fraction profile:

$$G(Z,\xi) = \delta(Z)Q(\xi). \quad (15)$$

Collocation with $n = 2$, and elimination of the wall concentration through the boundary condition in Eq. 8, yields an initial-value problem for the nodal functions $\tilde{C}_\infty(\tau,Z,\xi_1) \equiv \tilde{C}_{1\infty}(\tau,Z)$ and $\tilde{C}_\infty(\tau,Z,\xi_2) \equiv \tilde{C}_{2\infty}(\tau,Z)$. The boundary condition in Eq. 9, and the radial symmetry of the true solution, are satisfied through the use of only even powers of ξ in the collocation basis functions (Eq. 3). In place of Eq. 10 we then obtain

$$s\bar{\bar{\tilde{C}}}_{i\infty} + pV_i\bar{\bar{\tilde{C}}}_{i\infty} = \sum_{k=1}^{2} B'_{ik}\bar{\bar{\tilde{C}}}_{k\infty} + Q_i \quad i = 1,2 \quad (16)$$

in which V_i and Q_i are the given nodal values of $V(\xi)$ and $Q(\xi)$. To complete the solution, we compute the coefficients $B'_{11} = B'_{22} = -8$ and $B'_{12} = B'_{21} = 8$ from Eqs. 5 and 8, with the Gaussian nodes

$$\xi_1^2 = \frac{1}{2} - \frac{1}{\sqrt{12}}$$

$$\xi_2^2 = \frac{1}{2} + \frac{1}{\sqrt{12}} \quad (17)$$

and invert the transforms. The solution differs from zero only within the region $|Z_s| \leq |T|$, and is given there by

$$\tilde{C}_{1\infty} = \exp(-8\tau)\left\{\frac{Q_1\beta|T + Z_s|I_1(X)}{2X} + \frac{8Q_2I_0(X)}{|V_1 - V_2|} + Q_1\delta(Z_s - T)\right\} \quad (18.1)$$

$$\tilde{C}_{2\infty} = \exp(-8\tau)\left\{\frac{Q_2\beta|T - Z_s|I_1(X)}{2X} + \frac{8Q_1I_0(X)}{|V_1 - V_2|} + Q_2\delta(Z_s + T)\right\} \quad (18.2)$$

in which

$$Z_s = Z - (V_1 + V_2)\tau/2 \quad (19)$$

$$T = (V_1 - V_2)\tau/2 \quad (20)$$

$$\beta = 256(V_1 - V_2)^{-2} \quad (21)$$

$$X = \sqrt{\beta(T^2 - Z_s^2)}. \quad (22)$$

Interpolating the solution for $\tilde{C}$ according to Eq. 2, and integrating over the tube cross-section, we find the mean value to be $(\tilde{C}_{1\infty} + \tilde{C}_{2\infty})/2$. Gaussian quadrature over the cross-section gives the same result.

This completes the two-point collocation solution of Eqs. 6–9 in the nonreactive case. Approximate profiles of higher order are computable only numerically, and will be presented below. Analytic solutions are obtainable, however, for the axial moments of the collocation solution at any order n. In the next two sections, we test the convergence of the approximate moments so obtained, by comparison with known exact solutions.

CENTRAL MOMENTS OF THE TWO-POINT SOLUTION

Let $C(\tau,Z,\xi)$ be the solution of Eqs. 6–9 and 15 with $K'' = K''' = 0$, for any given value of the Peclet number. The mean mass fraction in a cross-section is defined, for these axisymmetric problems, by

$$\langle C \rangle = 2 \int_0^1 C\xi d\xi. \tag{23}$$

The central axial moments of $\langle C \rangle$ are

$$\mu_i = \int_{-\infty}^{\infty} (Z - \langle V \rangle \tau)^i \langle C \rangle dZ \tag{24}$$

and have the moment-generating function

$$\mu_i = (-\partial/\partial p)^i \{\exp(\langle V \rangle \tau p) \langle \overline{C}(\tau,p,\xi) \rangle\}|_{p=0} \tag{25}$$

in which $\overline{C}(\tau,p,\xi)$ is the Fourier transform of $C(\tau,Z,\xi)$.

For the collocation solution in Eqs. 18.1 and 18.2 corresponding operations give the central moments

$$\tilde{\mu}_0 = \frac{1}{2}(Q_1 + Q_2) \tag{26}$$

$$\tilde{\mu}_1 = (Q_1 - Q_2)(V_1 - V_2)\left[\frac{1 - \exp(-16\tau)}{64}\right] \tag{27}$$

$$\tilde{\mu}_2 = \tilde{\mu}_0 \left\{\frac{2\tau}{Pe^2} + \frac{(V_1 - V_2)^2}{8}\left[\frac{\tau}{4} - \frac{1 - \exp(-16\tau)}{64}\right]\right\} \tag{28}$$

as functions of the velocities V_i and pulse strengths Q_i at the collocation points.

For a radially uniform pulse of unit strength, Q_i is unity; and for developed laminar flow of a Newtonian fluid, $V_i = 1 - \xi_i^2$. Eqs. 26–28 then give

$$\tilde{\mu}_0 = 1 \tag{29}$$

$$\tilde{\mu}_1 = 0 \tag{30}$$

$$\tilde{\mu}_2 = \left(\frac{1}{Pe^2} + \frac{1}{192}\right)2\tau - \frac{1 - \exp(-16\tau)}{1536}. \tag{31}$$

The exact solutions derived by Aris (1956), Gill and Sankarasubramanian (1970), and Chatwin (1977) for a radially uniform pulse confirm Eqs. 29 and 30. Their expressions for μ_2 can be reduced (after a sign correction in Aris' solution) to the common form

$$\mu_2 = \left(\frac{1}{Pe^2} + \frac{1}{192}\right)2\tau - \frac{1}{1{,}440} + 32 \sum_{j=1}^{\infty} \lambda_j^{-8} \exp(-\lambda_j^2 \tau) \tag{32}$$

in which λ_j is the jth zero of the Bessel function $J_1(x)$. The terms porportional to τ constitute the prediction of the radially averaged Fickian dispersion model, with the long-time asymptotic dispersion coefficient found by Taylor (1953) and extended by Aris (1956). For brevity, this commonly-used model is called the Taylor-Aris model.

Before testing these results numerically, we give collocation solutions of higher order for the axial moments of the function $C(\tau,Z,\xi)$.

COLLOCATION SOLUTIONS OF HIGHER ORDER

The moments of the mass fraction profile about the origin are defined by

$$m_i(\tau,\xi) = \int_{-\infty}^{\infty} Z^i \omega(\tau,Z,\xi) dZ. \tag{33}$$

These moments can be obtained from the generating function

$$m_i(\tau,\xi) = (-\partial/\partial p)^i [\overline{\omega}(\tau,p,\xi)]|_{p=0} \tag{34}$$

without solving for the mass fraction profile. The moments at finite Pe can be obtained from those at infinite Pe by use of Eqs. 13 and 34.

A collocation solution for $m_i(\tau,\xi)$ at $Pe = \infty$ is obtained as follows. Let $\tilde{m}_i$ be the vector of mesh-point values of $\tilde{m}_i(\tau,\xi)$:

$$\tilde{\mathbf{m}}_i = [\tilde{m}_i(\tau,\xi_1), \cdots, \tilde{m}_i(\tau,\xi_n)]^T. \tag{35}$$

TABLE 1. SECOND MOMENT $1{,}000\left(\mu_2 - \frac{2\tau}{Pe^2}\right)$ FOR INITIAL CONDITION $G = \delta(Z)$

τ	Collocation $n = 2$	$n = 3$	$n = 4$	Exact*	Taylor-Aris
0.01	0.00791	0.00782	0.00780	0.00779	0.1042
0.05	0.1623	0.1575	0.1574	0.1574	0.5208
0.10	0.5221	0.5059	0.5059	0.5059	1.042
0.15	0.9705	0.9441	0.9442	0.9442	1.562
0.20	1.459	1.425	1.425	1.425	2.083
0.25	1.965	1.927	1.927	1.927	2.604
0.40	3.517	3.474	3.474	3.474	4.167
1.00	9.766	9.722	9.722	9.722	10.42

* Exact values are calculated from Eq. 32. The first two moments agree for all three methods.

TABLE 2. FIRST MOMENT $100\,\mu_1$ FOR INITIAL CONDITION $G = 2\xi^2\delta(Z)$

τ	Collocation $n = 2$	$n = 3$	$n = 4$	Exact*
0.01	−0.1540	−0.1516	−0.1511	−0.1511
0.05	−0.5736	−0.5540	−0.5541	−0.5541
0.10	−0.8314	−0.8083	−0.8086	−0.8086
0.15	−0.9472	−0.9298	−0.9299	−0.9299
0.20	−0.9992	−0.9880	−0.9880	−0.9880
0.25	−1.0226	−1.0160	−1.0159	−1.0159
0.40	−1.0399	−1.0388	−1.0388	−1.0388
1.00	−1.0417	−1.0417	−1.0417	−1.0417

* Exact values are calculated from Chatwin (1977). The first moment is independent of Pe, in view of Eqs. 13 and 34.

TABLE 3. SECOND MOMENT $1{,}000\left(\mu_2 - \frac{2\tau}{Pe^2}\right)$ FOR INITIAL CONDITION $G = 2\xi^2\delta(Z)$

τ	Collocation $n = 2$	$n = 3$	$n = 4$	Exact*
0.01	0.00791	0.00747	0.00738	0.00737
0.05	0.1623	0.1390	0.1389	0.1389
0.10	0.5221	0.4434	0.4447	0.4447
0.15	0.9705	0.8415	0.8431	0.8431
0.20	1.459	1.294	1.296	1.296
0.25	1.965	1.778	1.779	1.779
0.40	3.517	3.305	3.305	3.305
1.00	9.766	9.549	9.549	9.549

* Exact values are calculated from Chatwin (1977).

We apply the Fourier transformation and n-point radial orthogonal collocation to Eqs. 6–9 with $K'' = K''' = 0$ and $Pe = \infty$. Then by use of Eq. 34 we obtain the linear equation system

$$\frac{\partial}{\partial \tau}\tilde{\mathbf{m}}_i = \mathbf{B}'\tilde{\mathbf{m}}_i + i\,\mathbf{V}\tilde{\mathbf{m}}_{i-1}, \tag{36}$$

which can be solved directly for the moments up to any desired order N, given the initial vectors $\mathbf{m}_0, \cdots, \mathbf{m}_N$. Eqs. 13, 34, and 36 can then be used to obtain the moments at finite values of Pe. Finally, the cross-sectional averages $\langle \tilde{\mathbf{m}}_i \rangle$ can be obtained by Gaussian quadrature, and from these the central moments $\tilde{\mu}_1, \ldots, \tilde{\mu}_N$ are readily calculated.

Tables 1, 2 and 3 show the collocation solutions and the exact solutions for μ_0, μ_1, and μ_2 for two initial solute distributions. The collocation solutions converge rapidly with increasing n for all values of τ, and for both initial distributions. From Table 1 we see that the collocation solution for $n = 2$ is particularly accurate in the case of a uniform initial radial distribution.

TWO-DIMENSIONAL INITIAL DISTRIBUTIONS

Any axially symmetric initial distribution can be expressed in the form

$$G(Z,\xi) = \sum_j \sum_k b_{jk}\varphi^j(Z)Q^k(\xi) \tag{37}$$

with suitable basis functions $\varphi^j(Z)$ and $Q^k(\xi)$. Let $C^k(\tau,Z,\xi)$ be the solution of Eqs. 6–9 with constant K'' and K''', and with the initial distribution $C^k(0,Z,\xi) = \delta(Z)Q^k(\xi)$. Then the solution corresponding to the initial condition in Eq. 37 is obtainable by superposition,

$$\omega(\tau,Z,\xi) = \sum_j \sum_k b_{jk} \int_{-\infty}^{\infty} \varphi^j(X)C^k(\tau,Z-X,\xi)dX \qquad (38)$$

and has the Fourier transform

$$\overline{\omega}(\tau,p,\xi) = \sum_j \sum_k b_{jk}\overline{\varphi}^j(p)\overline{C}^k(\tau,p,\xi). \qquad (39)$$

Let Φ_i^j and M_i^k be the ith moments of the functions $\varphi^j(Z)$ and $C^k(\tau,Z,\xi)$ respectively with respect to Z. Then from Eqs. 34 and 39 we get the moments m_i in the form

$$m_i(\tau,\xi) = \sum_j \sum_k b_{jk} \sum_{r=0}^{i} \binom{i}{r} \Phi_{i-r}^j M_r^k(\tau,\xi) \qquad (40)$$

for any initial distribution of the form in Eq. 37. This result shows the influence of the initial conditions on the moments of the mass fraction profile at any later time.

PROFILES FOR A PULSE OF FINITE LENGTH

As a further test of the collocation solutions, we calculate the mass fraction profiles for an initial pulse of maximum amplitude unity and of finite length L equal to 0.1 unit of Z. To facilitate finite-element analysis, we introduce the coordinate

$$U = (2Z - \tau)/(L + \tau) \qquad (41)$$

and choose the initial distribution

$$G(Z,\xi) = \varphi(U) \qquad (42)$$

in which $\varphi(U)$ is a piecewise polynomial:

$$\left.\begin{aligned} &\varphi(U) = 1 \qquad \text{for } |U| \leq 0.975 \\ &\varphi(U) = 1 - 3\left(\frac{|U| - 0.975}{0.025}\right)^2 + 2\left(\frac{|U| - 0.975}{0.025}\right)^3 \\ &\qquad\qquad\qquad \text{for } 0.975 \leq |U| \leq 1 \\ &\varphi(U) = 0 \qquad \text{for } |U| \geq 1 \end{aligned}\right\} \qquad (43)$$

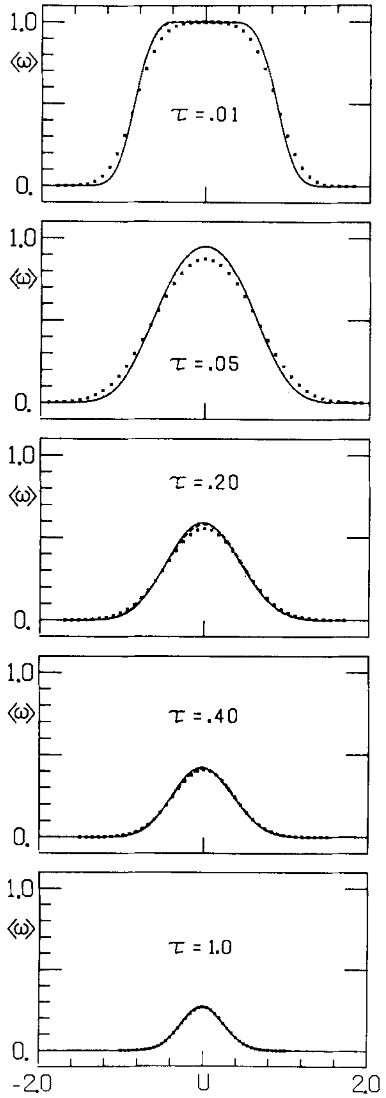

Figure 1. Radially averaged profiles at Pe = 15, for the initial condition of Eqs. 42–43.

——— Reference solution by finite elements

- - - - Collocation solution with n = 2

x x x x Solution by Taylor-Aris model

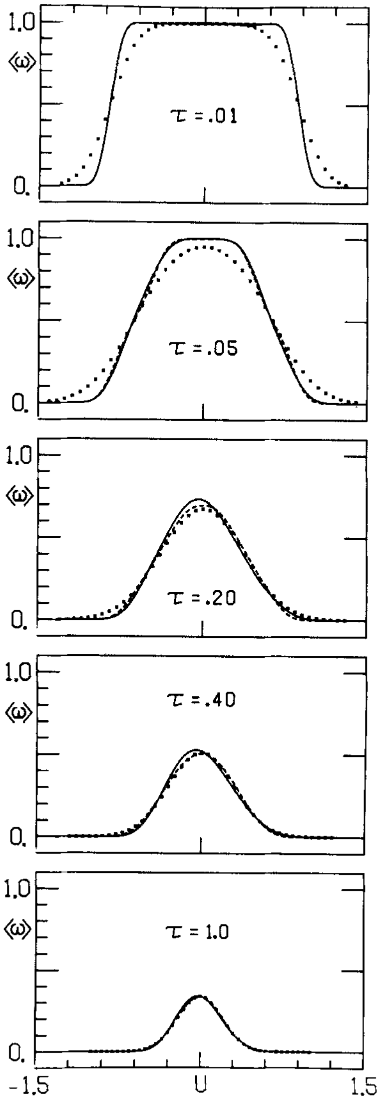

Figure 2. Radially averaged profiles at Pe = 40, for the initial condition of Eqs. 42–43.

——— Reference solution by finite elements

- - - - Collocation solution with n = 2

x x x x Solution by Taylor-Aris model

With this nearly rectangular initial distribution, the solution $\omega_\infty(\tau,Z,\xi)$ [obtained by neglecting longitudinal molecular diffusion] is permanently zero outside the region $-1 \leq U \leq 1$.

Figures 1, 2 and 3 show the cross-sectional average mass fraction $\langle\omega\rangle$ as a function of τ and z at $Pe = 15$, 40, and infinity. Three methods of solution are shown: orthogonal collocation on finite elements of U, two-point radial collocation, and the Taylor-Aris model. The radial collocation was done in all cases as described above; the finite elements were defined on cylinders of radius unity and length $\Delta U = 0.025$, using quartic polynomials in ξ^2 and cubic splines in U. Each method was first applied with $Pe = \infty$, and Eq. 14 was then used to get results at finite Peclet numbers. The two-point collocation profiles (dashed curves) model the true solutions very well, except for some lack of smoothness at short times with $Pe = \infty$. The Taylor-Aris model exaggerates the width of the tails of the pulse in every case.

For this radially uniform initial condition, the results of Gill and Sankarasubramanian (1970) agree closely with our finite-element calculations. A radially nonuniform pulse would provide a stricter comparison, since in that case Gill and Sankarasubramanian (1971) predict concentration profiles symmetric in U, whereas Eqs. 18.1 and 18.2 predict asymmetry whenever $Q_1 \neq Q_2$.

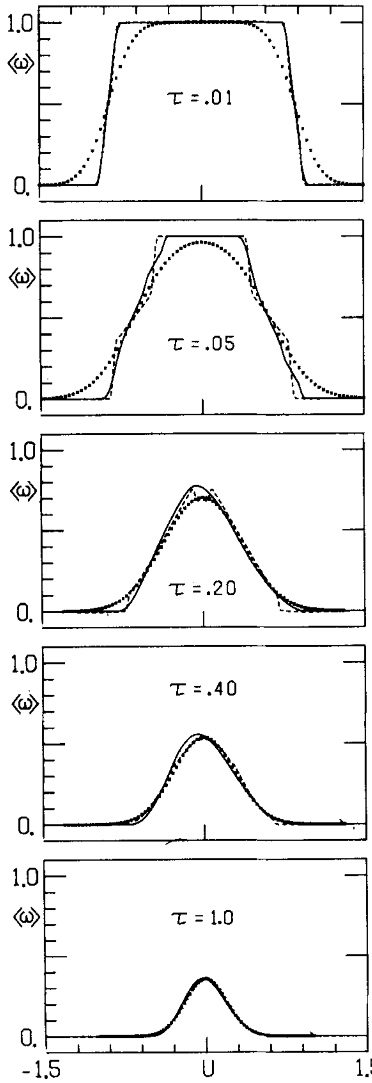

Figure 3. Radially averaged profiles at $Pe = \infty$, for the initial condition of Eqs. 42–43.

——— Reference solution by finite elements

- - - - Collocation solution with $n = 2$

x x x x Solution by Taylor-Aris model

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NOTATION

A_{ik}	= coefficients for gradient operator in Eq. 4
a_{im}, b_{jk}	= coefficients of basis functions
B_{ik}	= coefficients for Laplacian operator in Eq. 5
B'_{ik}	= coefficients for Laplacian operator with boundary point eliminated
$\mathbf{B}'$	= matrix of order n with elements B'_{ik}
C	= solution of Eqs. 6–9 and 15 with vanishing K'' and K'''
C^k	= special form of C for initial solute distribution $\delta(Z)Q^k(\xi)$
C_∞	= limit of C as $Pe \to \infty$
$\mathcal{D}_{AB}$	= binary diffusivity, $m^2\ s^{-1}$
$G(\xi,Z)$	= initial solute mass-fraction distribution, Eq. 7
$I_n(X)$	= modified Bessel function of the first kind
K'''	= $k'''R^2/\mathcal{D}_{AB}$, first Damköhler number
K''	= $k''R/\mathcal{D}_{AB}$, second Damköhler number
k'''	= rate coefficient for homogeneous first-order chemical reaction, s^{-1}
k''	= rate coefficient for heterogeneous first-order chemical reaction, $m\ s^{-1}$
m_i	= ith axial moment of ω defined in Eq. 33
$\mathbf{m}_i$	= vector of nodal values of m_i, Eq. 35
n	= number of radial collocation points interior to $\xi = 1$
p	= Fourier transform variable
Pe	= $RV_{max}/\mathcal{D}_{AB}$, Peclet number
$Q(\xi)$	= radial function in initial condition of Eq. 15
Q_i	= value of $Q(\xi)$ at ith collocation point
$Q^k(\xi)$	= kth radial basis function in initial condition of Eq. 37
R	= tube radius, m
r	= radial coordinate, m
s	= Laplace transform variable
t	= time, s
U	= transformed axial coordinate in Eq. 41
$V(\xi)$	= velocity profile, relative to centerline value
V_i	= value of $V(\xi)$ at ith collocation point
V_{max}	= maximum velocity in tube, $m\ s^{-1}$
$\mathbf{V}$	= diagonal matrix with elements $V_{ii} = V_i$
Y_m	= mth state variable (e.g., temperature or species mass fraction)
z	= axial coordinate, m
Z	= $z\mathcal{D}_{AB}/(V_{max}R^2)$, dimensionless axial coordinate
Z_s	= shifted dimensionless axial coordinate in Eq. 19

Greek Letters

$\delta(x)$	= unit impulse function
μ_i	= ith central moment of C defined in Eq. 24
ξ	= r/R, dimensionless radial coordinate
τ	= tD_{AB}/R^2, dimensionless time
$\varphi(U)$	= axial function in initial condition of Eq. 43
$\varphi^j(Z)$	= jth axial basis function in initial condition of Eq. 37
ω	= solute mass fraction

Symbols

$\bar{f}$	= Fourier transform of f
$\bar{\bar{f}}$	= Laplace transform of $\bar{f}$

f = approximate solution for indicated function, based on Eq. 1
⟨ ⟩ = average over flow cross-section
$\binom{i}{r}$ = binomial coefficient

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Particulate Deposition from Turbulent Parallel Streams

A theory is developed for the rate of particulate deposition from turbulent gas streams onto surfaces. Three characteristic times—the particle relaxation time, the turbulent fluctuation time, and the particle residence time—control the deposition mode. Two phenomena are primarily responsible for transport of the particles across the laminar sublayer and deposition: 1) the momentum imparted to the particle by the fluid turbulence; and 2) the thermospheresis caused by the temperature gradient near the wall. Interaction of the three characteristic times with these two phenomena is analyzed, and the particle deposition rate in turbulent pipe flow is computed. The findings are found to be in close agreement with available experimental data.

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SCOPE

Successful design of much industrial equipment such as certain heat exchanger surfaces requires understanding the mechanisms of mass transfer from the particle- or droplet-laden gas streams to solid surfaces. Particulate (or droplet) deposition on surfaces is caused by three different mechanisms, depending largely on the particle relaxation time and the turbulent fluctuation time. The particle relaxation time is proportional to the square of the particle diameter and to the material density of the particle, and is inversely proportional to the fluid viscosity. The very large particles, for which the relaxation time is much longer than the turbulent fluctuation time, impinge on surfaces that cross their mean trajectories. Therefore, in a parallel flow, capture of these particles is rare.

Smaller particles, for which the relaxation time is of the order of or smaller than the turbulent fluctuation time, diffuse across the mean streamlines toward the wall because of the fluid turbulence. The larger particles among these, for which the relaxation time is of the order of the turbulent fluctuation time, gain sufficient turbulence momentum to carry them across the laminar sublayer and result in wall deposition. For the particle material densities of the order of 2,000 kg/m^3, these particles are approximately 1 to 10 μm in radius when the air is used as a carrier gas.

The momentum of the smaller particles, with relaxation time much smaller than the fluctuation time, dissipates in the sublayer; it is not sufficient to result in their capture on the wall. There are two phenomena that could extend the particulate migration to the wall; the Brownian motion and thermophoresis. The Brownian motion is inefficient; its contribution to the deposition can be neglected for all practical purposes (Fuchs, 1964). On the other hand, thermophoresis is an effective mechanism that causes diffusion of the submicron particles toward the colder surface when a temperature gradient is imposed across the laminar sublayer.

In the following, a theoretical model is constructed that describes the transport of particles from turbulent streams to

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