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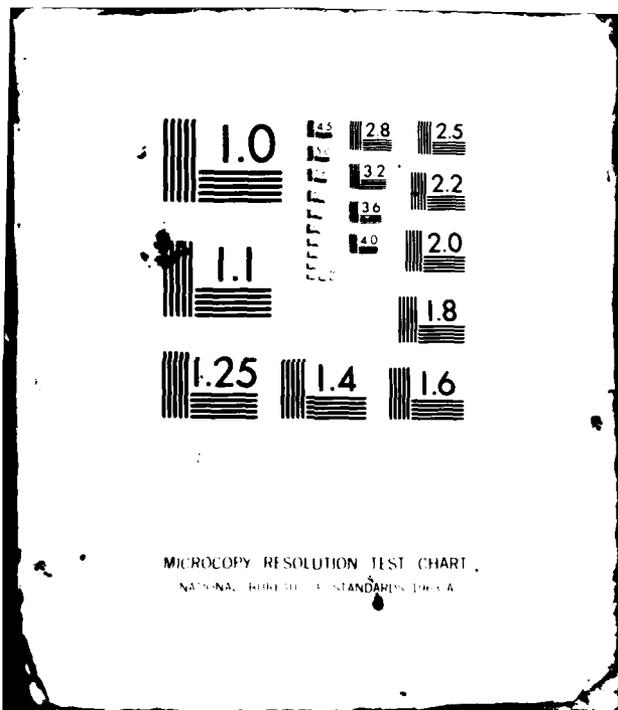
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NEW DESCRIPTIONS OF DISPERSION IN
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CONVOLUTION AND COLLOCATION METHODS

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NEW DESCRIPTIONS OF DISPERSION IN FLOW THROUGH TUBES:
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ABSTRACT

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 direction. 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 obtained at this level of approximation.

AMS (MOS) Subject Classifications: 35A35, 41A10, 41A63, 44A30, 65N35, 65N40,
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Key Words: Dispersion, Diffusion, Polynomial approximation, Orthogonal
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NEW DESCRIPTIONS OF DISPERSION IN FLOW THROUGH TUBES:
CONVOLUTION AND COLLOCATION METHODS

James C. Wang and Warren E. Stewart

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 \bar{Y}_m in the form

$$\bar{Y}_m = \sum_{i=0}^n a_{im}(\tau, Z) \xi^{2i} \quad 0 < \xi < 1 \quad (1)$$

This expansion can also be written as a Lagrange polynomial

$$\bar{Y}_m = \sum_{k=1}^{n+1} w_k(\xi) \bar{Y}_m(\tau, Z, \xi_k) \quad 0 < \xi < 1 \quad (2)$$

with radial basis functions

$$w_k(\xi) = \prod_{j \neq k} (\xi^2 - \xi_j^2) / \prod_{j \neq k} (\xi_k^2 - \xi_j^2) \quad (3)$$

Thus, each approximate profile \bar{Y}_m is represented by Lagrange interpolation in terms of its values $\bar{Y}_m(\tau, Z, \xi_k)$ at a set of chosen radial nodes ξ_k . We choose ξ_1^2, \dots, ξ_n^2 as the zeros of the shifted Legendre polynomial $P_n(x)$ (Abramowitz and Stegun, 1972) and choose ξ_{n+1} as the wall location, $\xi = 1$.

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

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

$$\begin{aligned} \frac{1}{\xi} \frac{d}{d\xi} \left(\xi \frac{d\bar{Y}_m}{d\xi} \right) \Big|_{\tau, Z, \xi_i} &= \sum_{k=1}^{n+1} \left[\frac{1}{\xi} \frac{d}{d\xi} \left(\xi \frac{dW_k}{d\xi} \right) \Big|_{\xi_i} \right] \bar{Y}_m(\tau, Z, \xi_k) \\ &= \sum_{k=1}^{n+1} B_{ik} \bar{Y}_{mk}(\tau, Z) \end{aligned} \quad (5)$$

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 \bar{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 non-linear. If they are linear, then $\bar{Y}_{m,n+1}$ can be expressed linearly in terms of the interior values \bar{Y}_{mk} by use of the boundary condition and Eq. (4). This permits elimination of $\bar{Y}_{m,n+1}$ from Eq. (5); the resulting new weight coefficients will be denoted by B'_{ik} . In non-linear cases, on the other hand, one retains the wall values as working variables and applies the boundary conditions numerically during 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 continuity equation for either species 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

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

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

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

Here K''' and K'' are the first and second dimensionless numbers of Damköhler (1936) for homogeneous and heterogeneous reactions. The Laplace-Fourier transform of Eqs. (6) - (9) from (τ, Z, ξ) into (s, p, ξ) is

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

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

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

Let Ω_∞ be the solution of Eqs. (6) - (9) with $Pe = \infty$. Its transform satisfies eqs. (10) - (12) with the p^2 term suppressed. Use of the s-shift theorem and Fourier convolution (Campbell and Foster 1967) then gives:

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

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

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

TWO-POINT COLLOCATION; NON-REACTIVE 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 (8), yields an initial-value problem for the nodal

functions $\bar{C}_\infty(\tau, Z, \xi_1) \equiv \bar{C}_{1\infty}(\tau, Z)$ and $\bar{C}_\infty(\tau, Z, \xi_2) \equiv \bar{C}_{2\infty}(\tau, Z)$. The boundary condition (9), and the symmetry of the true solution, are satisfied through the use of only even powers of ξ in the collocation basis functions [see Eq. (3)]. In place of Eq. (10) we then obtain

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

in which V_i and Q_i are the nodal values of $v(\xi)$ and $q(\xi)$. To complete the solution, we evaluate the coefficients B'_{ik} from Eqs. (5) and (8), with the Gaussian nodes

$$\left. \begin{aligned} \xi_1^2 &= \frac{1}{2} - \frac{1}{\sqrt{12}} \\ \xi_2^2 &= \frac{1}{2} + \frac{1}{\sqrt{12}} \end{aligned} \right\} \quad (17)$$

and invert the transforms. The solution differs from zero only within the region $|\tilde{Z}| < |T|$, and is given there by

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

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

in which

$$\tilde{Z} = Z - (V_1 + V_2)\tau/2 \quad (19)$$

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

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

$$x = \sqrt{\beta(T^2 - \tilde{Z}^2)} \quad (22)$$

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

CENTRAL MOMENTS OF THE TWO-POINT SOLUTION

Let C be the solution of Eqs. (6) - (9) and (15) with $K'' = K''' = 0$. The mean mass fraction in a cross-section is defined, for these axisymmetric problems, by

$$\langle C \rangle = 2 \int_0^1 C \xi d\xi \quad (23)$$

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

$$\mu_i = \int_{-\infty}^{\infty} (z - \langle v \rangle \tau)^i \langle C \rangle dz \quad (24)$$

and have the moment-generating function

$$\mu_i = \left(-\frac{d}{dp} \right)^i \left[\exp(\langle v \rangle \tau p) \langle \bar{C}(\tau, p, \xi) \rangle \right]_{p=0} \quad (25)$$

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

For the collocation solution with $n = 2$, we thus obtain

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

$$\bar{\mu}_1 = (Q_1 - Q_2)(v_1 - v_2) \left(\frac{1 - \exp(-16\tau)}{64} \right) \quad (27)$$

$$\bar{\mu}_2 = \bar{\mu}_0 \left\{ \frac{2\tau}{Pe^2} + \frac{(v_1 - v_2)^2}{8} \left(\frac{\tau}{4} - \frac{1 - \exp(-16\tau)}{64} \right) \right\} \quad (28)$$

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

$$\bar{\mu}_0 = 1 \quad (29)$$

$$\bar{\mu}_1 = 0 \quad (30)$$

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

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

$$\mu_2 = \left(\frac{1}{Pe} + \frac{1}{192}\right)2\tau - \frac{1}{1440} + 32 \sum_{j=1}^{\infty} \lambda_j^{-8} \exp(-\lambda_j^2 \tau) \quad (32)$$

in which λ_j is the j th zero of the Bessel function $J_1(x)$. The terms proportional to τ constitute the prediction of the standard Fickian dispersion model, with the long-time asymptotic dispersion coefficient found by Taylor (1953) and completed by Aris (1956). For brevity, the latter 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

$$m_i(\tau, \xi) = \int_{-\infty}^{\infty} z^i \Omega(\tau, z, \xi) dz \quad (33)$$

The generating function for these moments is

$$m_i(\tau, \xi) = \left(-\frac{d}{dp}\right)^i [\bar{\Omega}(\tau, p, \xi)] \Big|_{p=0} \quad (34)$$

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 \underline{m}_i be the vector of mesh-point values of $m_i(\tau, \xi)$:

$$\underline{m}_i = [m_i(\tau, \xi_1), \dots, m_i(\tau, \xi_n)]^T \quad (35)$$

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

$$\frac{\partial}{\partial \tau} m_i = B' m_i + i \sum m_{i-1} \quad (36)$$

Eqs. (13), (34), and (36) can then be used to obtain the moments at finite values of τ . Finally, the cross-sectional average $\langle m_i \rangle$ can be obtained by Gaussian quadrature of m_i .

Tables 1, 2, and 3 show the collocation solutions and the exact solutions for μ_0 , μ_1 , and μ_2 for two initial solution distributions. The collocation solutions converge rapidly toward the exact results 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

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

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

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

and has the Fourier transform

$$\bar{\Omega}(\tau, p, \xi) = \sum_j \sum_k b_{jk} \bar{\varphi}^j(p) \bar{C}^k(\tau, p, \xi) \quad (39)$$

Let Φ_i^j and M_i^k be the i th 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

Table 1 Second moment $1000(\mu_2 - \frac{2\tau}{Pe^2})$ for initial condition $\phi(\xi) = 1$

τ	Collocation			Exact *	Taylor-Aris
	n=2	n=3	n=4		
.01	.00791	.00782	.00780	.00779	.1042
.05	.1623	.1575	.1574	.1574	.5208
.10	.5221	.5059	.5059	.5059	1.042
.15	.9705	.9441	.9442	.9442	1.562
.20	1.459	1.425	1.425	1.425	2.083
.25	1.965	1.927	1.927	1.927	2.604
.40	3.517	3.474	3.474	3.474	4.167
1.0	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 $\phi(\xi) = 2\xi^2$

τ	Collocation			Exact*
	n=2	n=3	n=4	
.01	-.1540	-.1516	-.1511	-.1511
.05	-.5736	-.5540	-.5541	-.5541
.10	-.8314	-.8083	-.8086	-.8086
.15	-.9472	-.9298	-.9299	-.9299
.20	-.9992	-.9880	-.9880	-.9880
.25	-1.0226	-1.0160	-1.0159	-1.0159
.40	-1.0399	-1.0388	-1.0388	-1.0388
1.0	-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 $1000(\mu_2 - \frac{2\tau}{Pe^2})$ for initial condition $\phi(\xi) = 2\xi^2$

τ	Collocation			Exact*
	n=2	n=3	n=4	
.01	.00791	.00747	.00738	.00737
.05	.1623	.1390	.1389	.1389
.10	.5221	.4434	.4447	.4447
.15	.9705	.8415	.8431	.8431
.20	1.459	1.294	1.296	1.296
.25	1.965	1.778	1.779	1.779
.40	3.517	3.305	3.305	3.305
1.0	9.766	9.549	9.549	9.549

*Exact values are calculated from Chatwin (1977).

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

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 . The coordinate

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

is introduced here to facilitate finite element calculations of the solution. The following initial condition is used,

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

in which $\varphi(U)$ is a C^1 cubic spline:

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

With this initial condition, the solution C_∞ (valid for $Pe = \infty$) is permanently zero outside the region $-1 < U < 1$.

Figures 1, 2, and 3 show the cross-sectional average mass fraction $\langle w \rangle$ 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 of U were C^1 cubic splines with length $\Delta U = 0.025$. 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.

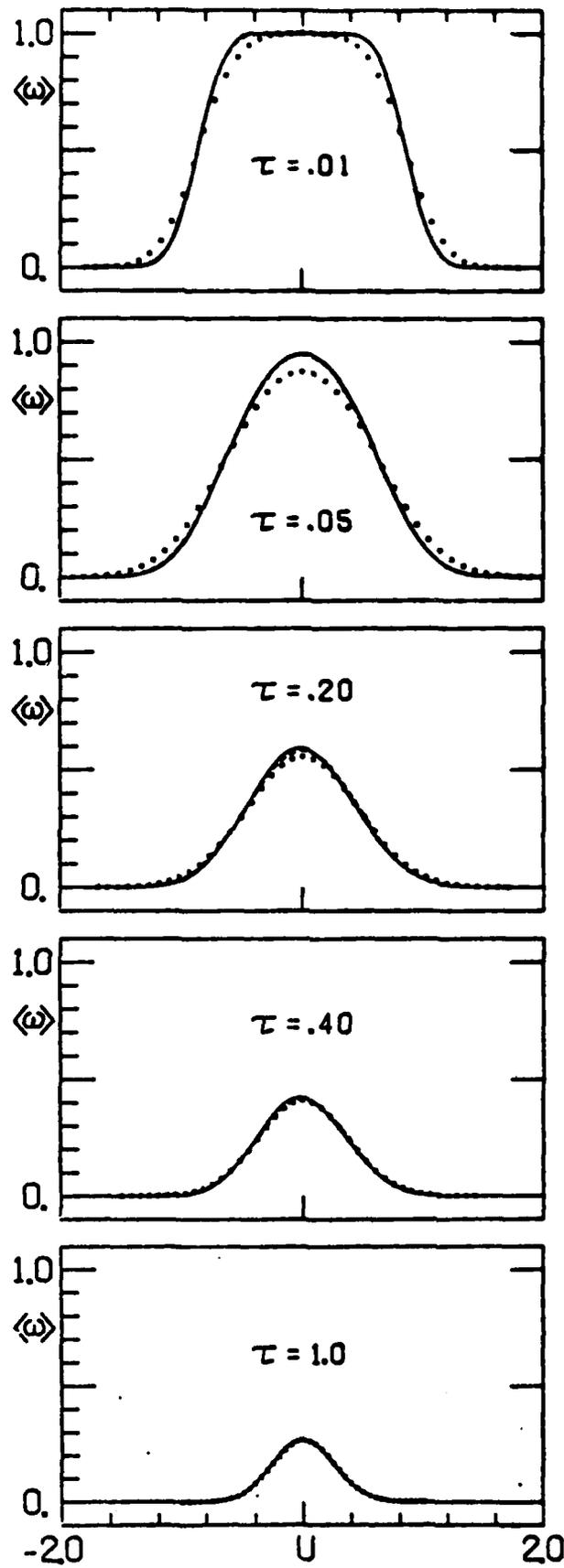


Figure 1. Radially averaged profiles at $Pe = 15$, for the initial condition of Eqs. (42)-(43).

— Reference solution by finite elements
 ---- Collocation solution with $n = 2$
 Solution by Taylor-Aris model

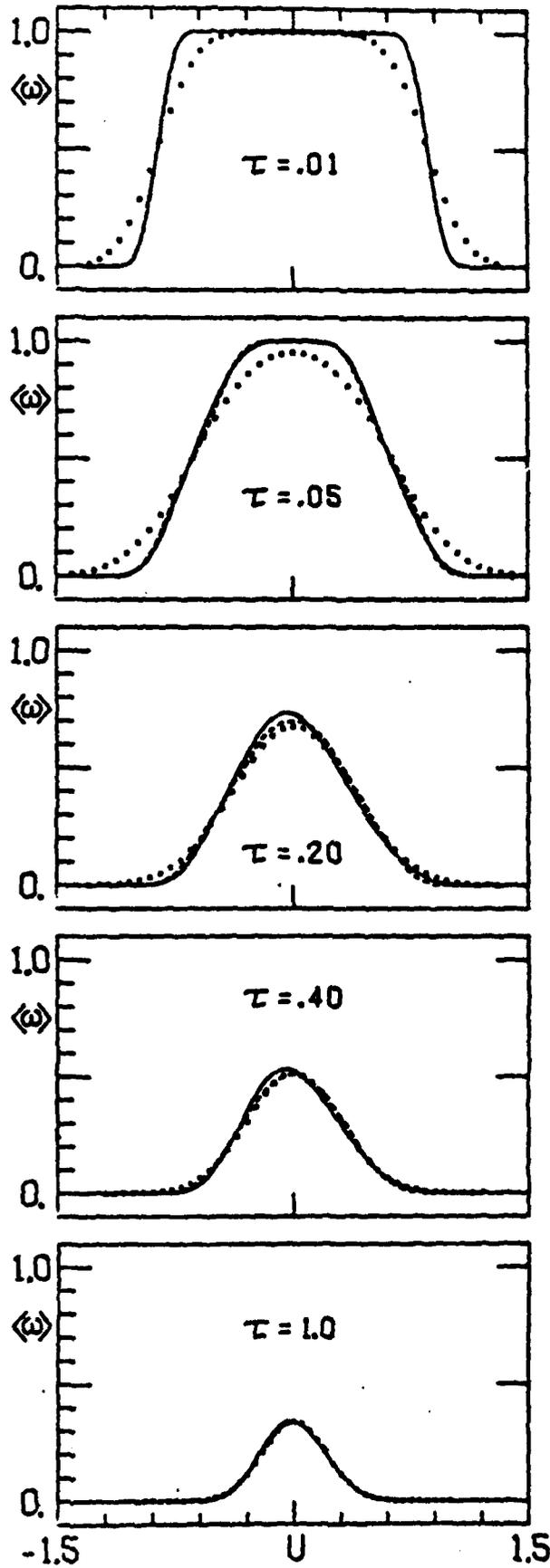


Figure 2. Radially averaged profiles at $Pe = 40$, for the initial condition of Eqs. (42)-(43)

- Reference solution by finite elements
- - - Collocation solution with $n = 2$
- Solution by Taylor-Aris model

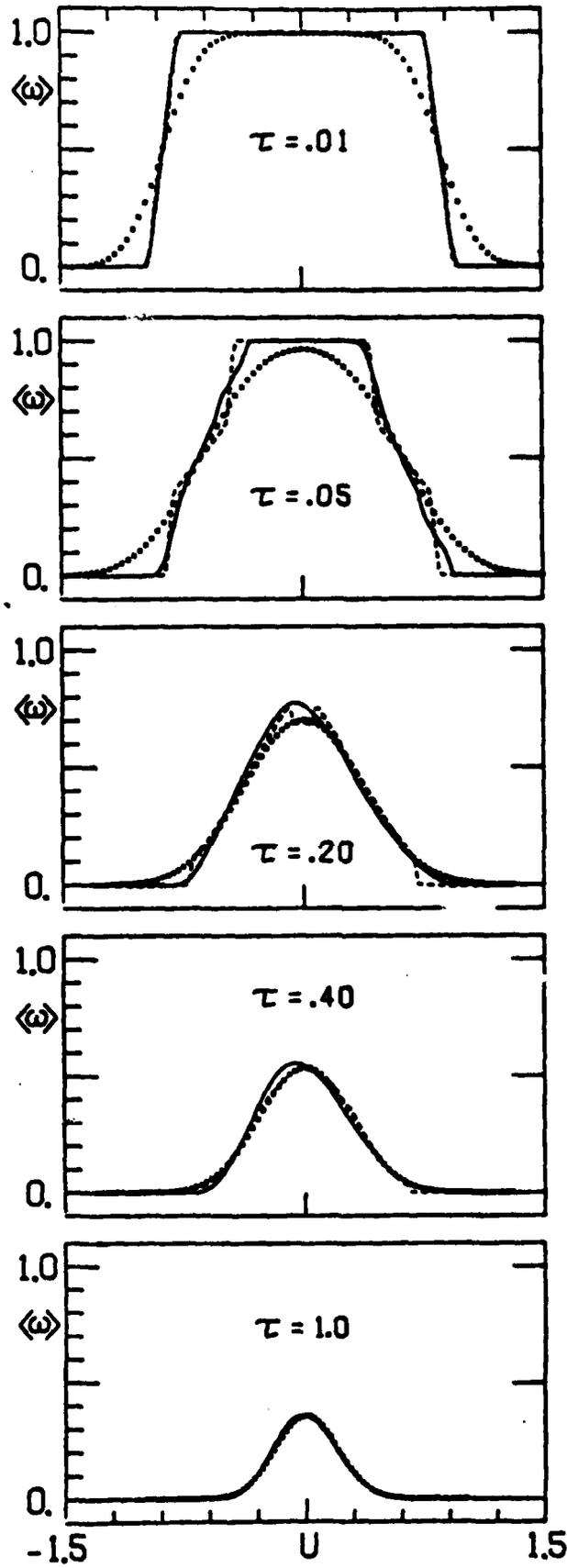


Figure 3. Radially averaged profiles at $Pe = \infty$, for the initial condition of Eqs. (42)-(43)

— Reference solution by finite elements
 - - - Collocation solution with $n = 2$
 Solution by Taylor-Aris model

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.

B' matrix of order n with elements B'_{ik}

C solution of Eqs. (6) - (9) with constant K'' and K''' and with initial condition $\delta(z)O(\xi)$

C^k special form of C for initial condition $\delta(z)O^k(\xi)$

C_∞ limit of C as $Pe \rightarrow \infty$

$G(\xi, z)$ initial distribution, Eq. (7)

$I_n(x)$ modified Bessel function of the first kind

K''', K'' first and second Damköhler numbers

m_i i th axial moment of Ω defined in Eq. (33)

\underline{m}_i vector of nodal values of m_i , Eq. (35)

n number of collocation points interior to $\xi = 1$

p Fourier transform variable

$Pe = RV_{\max}/D_{AB}$, Peclet number

$O(\xi)$ radial function in initial condition

O_i value of $O(\xi)$ at i th collocation point

$O^k(\xi)$ k th radial basis function in initial condition

s Laplace transform variable

U transformed Z coordinate in Eq. (41)

$v(\xi)$ velocity profile, relative to centerline value

v_i value of $v(\xi)$ at i th collocation point

V diagonal matrix with elements $V_{ii} = v_i$

Y_m mth state variable (e.g., temperature or species mass fraction)

$Z = z D_{AB} / (V_{\max} R^2)$, dimensionless axial coordinate

$\langle \rangle$ average over flow cross-section

$\binom{i}{r}$ binomial coefficient

Greek Letters

μ_i ith central moment of C defined in Eq. (24)

$\xi = r/R$, dimensionless radial coordinate

$\tau = t D_{AB} / R^2$, 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

Ω solution for ω with general initial condition $G(z, \xi)$

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) 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 con- volution of the profile for infinite Peclet number. Close approximations are ob- tained for the concentration profile and its axial moments, by use of orthogonal collocation in the radial direction. 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 prac- tical accuracy; analytical solutions are obtained at this level of approximation.		

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