BRIEF COMMUNICATION

CONVECTIVE DIFFUSION OF A SOLUTE IN PIPE FLOW

J. W. SHELDON,¹ K. A. HARDY¹ and P. KEHLER²

IPhysics Department, Florida International University, Miami, FL 33199, U.S.A. 2Argonne National Laboratory, Argonne, IL 60439, U.S.A.

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1. INTRODUCTION

A description of solute dispersion in pipe flow is provided by the solution to the convective diffusion equation. The solution to the convective diffusion problem presented herein is an application of work by Maron (1978). We present a solution to Maron's approximate equation by application of the Laplace transform with respect to time. Laplace and Fourier transforms have previously been applied to the advection diffusion equation for Poiseuille flow by Stokes & Barton (1985). They accomplished transform inversion by asymptotic evaluation of the poles to get approximate solutions near the leading and trailing fronts. Here we evaluate the inversion integral numerically.

The fluid can be a gas or liquid on laminar flow. We refer to the diffusing material as solute, though it could be an atomic, molecular or nuclear excited species of the bulk fluid. The solute concentration is described for aH times after injection and Maron's formalism allows for nonuniform solute injection and generalized velocity profiles. The concentration of solute at any time and position in the pipe is given in terms of an expansion about the mean concentration at any time and longitudinal position. Expansion coefficients are determined from the initial solute distribution and fluid velocity profile.

Consider a pipe of constant circular cross section whose axis is the z-axis of the (r, θ, z) cylindrical coordinate system. The local concentration of solute in the system is described by the convective diffusion equation with constant molecular diffusion coefficient D :

$$
\frac{\partial C'}{\partial t} + U(r, \theta) \frac{\partial C'}{\partial z} - D \left[\frac{\partial}{r \partial r} \left(r \frac{\partial C'}{\partial r} \right) + \frac{\partial^2 C'}{r^2 \partial \theta^2} + \frac{\partial^2 C'}{\partial z^2} \right] = -\frac{C'}{T_{\frac{1}{2}}},
$$
 [1]

where $C'(t, r, \theta, z)$ is the local solute concentration, $U(r, \theta)$ is the magnitude of the z-directed rectilinear flow velocity and $T_λ$ is the half-life of a radioactively decaying solute. The substitution $C' = C \exp(-t/T_k)$ is used to obtain an equation of the form of [1] for C but with the r.h.s. equal to zero. A coordinate system fixed in the frame of the pipe is used with the dimensionless variables $\eta = r/R$, $\xi = z/R$, $\tau = Dt/R^2$ and the dimensionless parameter $Y = U_0R/D$ (the Peclet number, $Pe=2Y$). Here R is the pipe radius and U_0 is the mean velocity of the flow with a local dimensionless profile given by $Y\Phi(\eta, \theta)$. Defining the cross-sectional mean

$$
\overline{C}(\tau,\zeta)=\frac{1}{\pi}\int_0^{2\pi}\int_0^1 C(\tau,\eta,\theta,\zeta)\eta\;d\eta\;d\theta,\qquad [2]
$$

Maron obtained

$$
\frac{\partial \overline{C}}{\partial \tau} + Y \frac{\partial \overline{C}}{\partial \xi} - \left(1 + \frac{Y^2}{\pi} \sum_{n=1}^{\infty} \sum_{\gamma=0}^{\infty} \frac{a_m^2}{\lambda_m^2 N_m} \right) \frac{\partial^2 \overline{C}}{\partial \xi^2} - Y \sum_{n=1}^{\infty} \sum_{\gamma=0}^{\infty} \frac{a_m}{N_m} \frac{\partial u_m^0}{\partial \xi} \exp(-\lambda_m^2 \tau) \n- \frac{Y^2}{\pi} \sum_{n=1}^{\infty} \sum_{\gamma=0}^{\infty} \frac{a_m^2}{\lambda_m^2 N_m} \frac{\partial}{\partial \tau} \int_0^{\tau} \frac{\partial^2 \overline{C}(\tau', \xi)}{\partial \xi^2} \exp[-\lambda_m^2 (\tau - \tau')] d\tau', \quad [3]
$$

where

$$
a_{\sigma m} = \int_0^{2\pi} \int_0^1 \left[\Phi(\eta, \theta) - 1 \right] \chi_{\sigma m}(\eta, \theta) \eta \, d\eta \, d\theta, \tag{4}
$$

$$
u_{\sigma m}^{0}(\xi) = \int_{0}^{2\pi} \int_{0}^{1} C(0, \eta, \theta, \xi) \chi_{\sigma m}(\eta, \theta) \eta \, d\eta \, d\theta \qquad [5]
$$

and

$$
N_{\gamma n} = \int_0^{2\pi} \int_0^1 \chi_{\gamma n}^2 \eta, d\eta d\theta, \qquad [6]
$$

with $\chi_{m} = \cos(\gamma \theta) J_{\gamma}(\lambda_{m} \eta)$, where J_{γ} is the γ -order Bessel function of the first kind and λ_{m} is the n th zero of its first derivative. Maron gives the local solute concentration as

$$
C(\tau, \eta, \theta, \xi) = \sum_{n=1}^{\infty} \sum_{\gamma=0}^{\infty} \frac{u_{\gamma n}^0(\xi)}{N_{\gamma n}} \chi_{\gamma n}(\eta, \theta) \exp(-\lambda_{\gamma n}^2 \tau)
$$

-
$$
Y \sum_{n=1}^{\infty} \sum_{\gamma=0}^{\infty} \frac{a_{\gamma n} \chi_{\gamma n}(\eta, \theta)}{N_{\gamma n}} \int_{0}^{\tau} \frac{\partial \overline{C}(\tau', \xi)}{\partial \xi} \exp[-\lambda_{\gamma n}^2(\tau - \tau')] d\tau' + \overline{C}(\tau, \xi). \quad [7]
$$

2. SOLUTION

The solution to [3] represents the axial and temporal dependence of the cross-sectional mean solute concentration. This result, with the a_{ν} s from the velocity profile and the u_{ν}^0 s obtained from the initial solute distribution, can be used in [7] to obtain the complete spacial and temporal dependence of the solute concentration at any downstream station.

The solution to [3] is obtained by performing the indicated differentiation of the last term and taking the Laplace transform with respect to τ to get

$$
pG(p,\xi)-\bar{C}_0(\xi)+Y\frac{\partial G(p,\xi)}{\partial \xi}=K(p)\frac{\partial^2 G(p,\xi)}{\partial \xi^2}-L(p)\frac{\partial \bar{C}_0(\xi)}{\partial \xi},\qquad [8]
$$

where

$$
G(p,\xi) = \int_0^\infty \overline{C}(\tau,\xi) \exp(p\tau) d\tau,
$$
 [9a]

$$
K(p) = 1 + \frac{Y^2}{\pi} \sum_{n=1}^{\infty} \sum_{\gamma=0}^{\infty} \frac{a_{\gamma n}^2}{N_{\gamma n}(p + \lambda_{\gamma n}^2)},
$$
 [9b]

$$
L(p) = \frac{Y}{\pi} \sum_{n=1}^{\infty} \sum_{\gamma=0}^{\infty} \frac{a_{\gamma n} A_{\gamma n}}{N_{\gamma n} (p + \lambda_{\gamma n}^2)}
$$
 [9c]

and

$$
u_{\gamma n}^0(\xi) = A_{\gamma n} \overline{C}_0(\xi). \tag{9d}
$$

 $\overline{C}_0(\xi)$ is the ξ dependence of the initial solute distribution and it has been assumed the ξ dependence of $C(0, \eta, \theta, \zeta)$ is separable from $H(\eta, \theta)$, the initial η and θ dependence, in writing [9d]. Using [5] **and [9d], one obtains**

$$
A_{\gamma n} = \int_0^{2\pi} \int_0^1 H(\eta, \theta) \chi_{\gamma n}(\eta, \theta) \eta \, d\eta \, d\theta. \qquad [10]
$$

The solution of [8] by variation of parameters can be put in the form

$$
G(p,\xi) = \frac{[1 - L(p)M_{+}(p)]\exp[M_{+}(p)\xi]}{K(p)[M_{+}(p) - M_{-}(p)]} \int_{\xi}^{\infty} C_{0}(\xi')\exp[-M_{+}(p)\xi'] d\xi',
$$

$$
+ \frac{[1 - L(p)M_{-}(p)]\exp[M_{-}(p)\xi]}{K(p)[M_{+}(p) - M_{-}(p)]} \int_{-\infty}^{\xi} C_{0}(\xi')\exp[-M_{-}(p)\xi'] d\xi', \quad [11]
$$

where

$$
M_{\pm}(p) = Y \pm \frac{[Y^2 + 4pK(p)]^{\frac{1}{2}}}{2K(p)}.
$$

For a slug of solute of mean concentration C_0 which initially extends from $-\xi_s/2$ to $+\xi_s/2$, one obtains

$$
G(p,\xi) = C_0 \left\{ \frac{1 - M_{-}(p)L(p)}{K(p)[M_{+}(p) - M_{-}(p)]} \right\} \left\{ \frac{2 \sinh \left[M_{-}(p) \frac{\xi_{s}}{2}\right]}{M_{-}(p)} \right\} \exp[M_{-}(p)\xi].
$$
 [12]

The inversion of [12] then finally gives the Bromwich integral:

$$
\overline{C}(\tau,\xi) = \frac{C_0}{2\pi i} \int_{a-i\infty}^{a+i\infty} \left\{ \frac{1 - M_{-}(p)L(p)}{K(p)[M_{+}(p) - M_{-}(p)]} \right\} \left\{ \frac{2 \sinh\left[M_{-}(p)\frac{\xi_{s}}{2}\right]}{M_{-}(p)} \right\} \exp[M_{-}(p)\xi + pt] dp. \quad [13]
$$

To facilitate the numerical integration of the real integral in [13] define $p = a + iy$, $q_1 = K(p)$, $q_2 = Y^2 + 4K(p)p$, $q_3 = L(p)$ and $q_4 = [\sinh(M - \xi_3/2)]/(M - \xi_3/2)$. Then using $q_j = r_j(\cos\theta_j + i \sin\theta_j)$ the real part of [13] can be put in the form

$$
\overline{C}(\tau,\xi) = \exp(at) \int_0^\infty \exp[\xi c_2(y)] \{c_1(y) \cos[\xi s_2(y) + ty - \theta_4] + s_1(y) \sin[\xi s_2(y) - ty - \theta_4] \} dy,
$$
\n[14a]

where

$$
\mathbf{c}_1(\mathbf{y}) = \left[\begin{array}{c} +\cos\left(\frac{\theta_2}{2}\right) - \left(\frac{\gamma r_3}{r_1}\right)\cos\left(\theta_3 - \theta_1 - \frac{\theta_2}{2}\right) + \left(\frac{r_3\sqrt{r_2}}{r_1}\right)\cos\left(\theta_3 - \theta_1\right) \end{array} \right] \frac{r_4}{(\pi\sqrt{r_2})} \quad [14b]
$$

and

$$
\begin{aligned} \mathcal{C}_2(y) &= \left[Y \frac{\cos}{\sin}(\theta_1) \mp \sqrt{r_2} \frac{\cos}{\sin}(\frac{\theta_2}{2} - \theta_1) \right]. \end{aligned} \tag{14c}
$$

For the limiting case of a pulse input, $\xi_s \rightarrow 0$, which gives $r_4 = 1$ and $\theta_4 = 0$ in [14a,b]. The computational procedure is to obtain the $a_{\sigma m}$ from [4] for a given flow profile, and the $A_{\gamma n}$ from [10] for the input slug's given radial and angular distribution. Using these results in [9b] and [9c] we obtain expressions for the r_is and θ_i s which appear in [14a-c]. The numerical integration of [14a] can then be carried out.

3. RESULTS

The numerical results reported here are for solute dispersion in pipe flow with a steady parabolic fluid velocity profile for which [4] reduces to

$$
a_{0n} = -\frac{8\pi}{\lambda_{0n}^2} J_0(\lambda_{0n})
$$

$$
a_{yn} = 0, \quad \gamma > 0.
$$

Figure 1. Cross-sectional mean temporal distribution of solute for Pe = 10. Initial conditions: $\zeta_s = 0.24$ and $\eta_0 = 1.0$. O, present results; \Box , computed from [34]-[36] of Gill & Sankarasubramanian (1971); numerical computation of Gill & Ananthakrishnan (1967). Axial stations: (a) $\xi = 0.5$; (b) $\xi = 2.5$; (c) $\xi = 8.0$.

The cases reported are chosen for comparison with results reported in the literature. The initial solute distribution is uniform over the dimensionless pipe length ζ_s centered at $\xi = 0$ and extends out to various dimensionless radii η_0 from 0.1 to 1.0. Numerical integrations are carried out using 5 terms in the summations in [9b] and [9c]. Extending the summation to 10 terms affects the reported results by <0.5%, except in the wings of the distribution in the $\eta_0 = 0.1$ case, for which the difference between 5 and 10 terms in the summations changed the results by up to 5%.

In figure 1 the mean concentration is displayed as a function of dimensionless time for an initially uniform solute distribution of unit concentration extending to the pipe wall at $n_0 = 1.0$ and of dimensionless length 0.24. Results are given for three detection stations located at dimensionless distances 0.5, 2.5 and 8.0. This choice of parameters allows comparison with the finite-difference calculations of Gill & Ananthakrishnan (1967). We also report points calculated using [34]-[36] of Gill & Sankarasubramanian (1971). There is general agreement between all three sets of results for this range of parameters.

Figure 2. Cross-sectional mean temporal distribution of solute for Pe = 2 at two axial stations. O, present results; computed from [34]-[36] of Gill & Sankarasubramanian (1971). Initial conditions: $\zeta_s = 0.25$; and (a) $\eta_0 = 0.1$, (b) $\eta_0 = 0.5$, (c) $\eta_0 = 1.0$.

A more extensive comparison with the work of Gill & Sankarasubramanian (1971) is presented in figure 2, where the initially uniform solute distribution extends over a dimensionless length of 0.25 and out to dimensionless radii $\eta_0 = 0.1$, 0.5 and 1.0. Two detection stations, one at $\zeta = 0.5$ and one at $\xi = 2.0$, are considered. Here there is excellent agreement between the present method and Gill & Sankarasubramanian (1971). The curves in figure 2 for the two detection stations are almost independent of the dimensionless radius of the initial solute distribution. This is due to the low Pe and the normalization of the detected mean concentration to the initial mean concentration $[C_0 = \overline{C}(0)]$. In Gill & Sankarasubramanian (1971, figure 7) a plot is given of $C(\tau, \xi = 200)$ for $\eta_0 = 1.0, 0.9, 0.7, 0.5$ and 0.3 with Pe = 1000. If these curves are normalized to \bar{C}_0 they have, within a few percent, the same peak value. Their peak positions in time are offset slightly with the initial distributions concentrated closest to the axis arriving first, This offset is not resolvable in the present case due to the low Pc.

4. CONCLUSIONS

The numerical integration of [14a] yields the cross-sectional average solute concentration at a dimensionless distance ζ downstream of the injection point at a dimensionless time τ . For low Pe, agreement with other work is demonstrated. The main advantage of the present method is the way in which the initial solute distribution enters the problem. The initial radial and angular distribution can be quite general, requiring only that the r and θ dependence is separable from the z dependence. Then the A_{ν} s can be computed from the integrals in [10]. The initial longitudinal distribution of solute used here applies only to the case of a slug or pulse input, however other longitudinal distributions could be introduced in the integral in [11].

One of the referees pointed out that Maron's equation could be applied to larger Pe if a moving frame of reference were adopted and the transform method of solution could still be used.

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