Contents lists available at ScienceDirect



International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt



Basic characteristics of Taylor dispersion in a laminar tube flow with wall absorption: Exchange rate, advection velocity, dispersivity, skewness and kurtosis in their full time dependance

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ARTICLE INFO

Article history: Received 26 November 2016 Received in revised form 25 January 2017 Accepted 17 February 2017 Available online 19 March 2017

Keywords: Taylor dispersion Wall absorption Concentration moments

1. Introduction

Taylor dispersion refers to solute transport in a confined flow under the combination of competing effects of longitudinal velocity nonuniformity and transverse diffusion. Velocity nonuniformity contributes mainly to the longitudinal spread of the cloud, while diffusion tends to smear out the transverse concentration nonuniformity [1]. With the effect of wall absorption, the dispersion process and corresponding solute distribution are reshaped essentially [2]. Taylor dispersion with wall absorption plays a central role in various applications such as contaminant dispersion in rivers and groundwater, and chemical engineering, and has attracted extensive studies [3–12].

For the problem of Taylor dispersion with wall absorption in a tube flow, there are five basic characteristic quantities as exchange rate, advection velocity, dispersivity, skewness and kurtosis, corresponding to the first five concentration moments, according to Sankarasubramanian and Gill [2] who originally explored the problem through a generalized dispersion model (Taylor-Gill approximation) [13–16]. The precise expression of exchange rate and asymptotically stationary values of advection velocity and dispersivity were derived and well illustrated. Solute is depleted under the effect of wall absorption and more concentrated in favor of

ABSTRACT

Taylor dispersion with wall absorption in a laminar tube flow is analytically studied in this work by Aris's method of concentration moments. The difficulty associated with the conventional approach initiated by Sankarasubramanian and Gill is completely avoided. All the basic characteristic properties governing the dispersion process, including the exchange rate, advection velocity, dispersivity, skewness and kurtosis, are analytically determined in their full time dependance for the first time. Detailed parametrical analysis is performed for the properties. Mean concentration distribution is concretely characterized.

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the central region where higher velocity increases the displacement and lower velocity gradient decreases the dispersion [2]. However, limited by the inherent complexity of series expansion, the advection velocity and dispersivity in their time dependance had not been captured, not to mention the mean concentration distribution in the early period. Extensive studies have then been made on the basic characteristic quantities and mean concentration [9,17,18,11,19–23]. Based on the Taylor-Gill approximation and by definition of different averages, Degance and Johns [17,18] gave complex expressions from which the advection velocity and dispersivity can be computed, but explicit mean concentration distribution were not illustrated owing to the slow convergence of proposed series. Further considering the effect of wall absorption upon mean concentration distribution, Smith [24] analyzed the evolution of asymptotically correct skewness by a delay-diffusion description associated with the mathematically preferred average identified by Degance and Johns [17,18]. For the Poiseuille flow, wall absorption was shown to reduce skewness or even to change the sign of skewness from positive to negative [24]. Other efforts also paid on the initial concentration distribution [25-27,5,7,28,29]. As a unique numerical study, Das and Mazumder [30] explored concentration moments through implicit finite-difference scheme, though failed to give the asymptotical dispersivity identical to that shown by Sankarasubramanian and Gill (Fig. 4) [2] and higher order characteristics identical to the result by Andersson and Berglin (Fig. 5) [31] for strong wall absorption. Till now, lower order characteristics have been substantially

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presented, leaving higher order characteristics including full time dependent skewness and kurtosis to be explored.

Skewness evaluates the degree of symmetry and kurtosis measures the degree of peakedness of the longitudinal distribution of mean concentration. Both approaches zero at large times as the mean concentration is then in Gaussian distribution [31,32]. Skewness and kurtosis are essential for characterizing the transitional phase prior to stationary asymptotics in dispersion process, and of great significance for selecting proper transport models for fractional dispersion [33] in modeling the probability density function of a diffusing scalar in atmospheric boundary layers [34] and exploring turbulent dispersion [35]. At the methodological level, higher order moments statistically contain accurate concentration information and can support other solution approaches [25,27–29,5,7]. It is therefore of fundamental importance to study the higher order moments to figure out the dispersion process.

Presented in this paper is a systematic study for Taylor dispersion with wall absorption in a tube flow, with full time dependent five characteristics and their absorption dependance completely derived and illustrated. The specific objectives of this paper are: (I) to introduce the method of moments and solve up to the fourth order moment; (II) to illustrate the full time evolutions of all the dispersion characteristics, with detailed parametrical analysis; and (III) to characterize the evolution of mean concentration distribution fitted by Hermite polynomials for the initial stage.

2. Formulation

Consider the scalar solute transport process in a fully developed steady laminar tube flow with a first-order wall absorption [2], the local concentration C^* of solute cloud satisfies the advection-diffusion equation as

$$\frac{\partial C^*}{\partial t} + u_0 \left(1 - \frac{r^2}{a^2} \right) \frac{\partial C^*}{\partial x} = D \frac{\partial^2 C^*}{\partial x^2} + D \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C^*}{\partial r} \right), \tag{2.1}$$

where t is the time, u_0 the centreline flow velocity, r the radial coordinate perpendicular to the tube axis, a the tube radius, x the longitudinal coordinate coinciding with the tube axis, and D the molecular diffusivity.

The initial condition is set as a uniform and instantaneous release of scalar substance with mass Q at the origin of coordinate x = 0 at time t = 0 as

$$C^*(0,x,r) = \frac{Q}{\pi a^2} \delta(x), \qquad (2.2)$$

where $\delta(x)$ is the Dirac delta function.

The boundary condition at the tube wall and symmetrical condition at the central axis read as

$$-D\frac{\partial C^*(t,x,a)}{\partial r} = \beta^* C^*(t,x,a), \quad \frac{\partial C^*(t,x,0)}{\partial r} = 0,$$
(2.3)

where β^* is the first-order wall absorption parameter.

Since the amount of released substance is finite, the upstream and downstream conditions are

$$C^*(t, \pm \infty, r) = 0.$$
 (2.4)

With dimensionless variables introduced as

$$\tau = \frac{Dt}{a^2}, \quad \eta = \frac{x - \overline{u}t}{a}, \quad \zeta = \frac{r}{a}, \quad C = \frac{\pi a^3}{Q}C^*,$$

$$Pe = \frac{\overline{u}a}{D}, \quad \psi = 1 - 2\zeta^2, \quad \beta = \frac{\beta^* a}{D},$$
(2.5)

where $\overline{u} = u_0/2$ is the mean velocity, with the overline indicating the operation of transverse average for a variable *f* defined as

$$\bar{f} \equiv \int_0^1 2\zeta f d\zeta. \tag{2.6}$$

Then the governing equation and the initial and boundary conditions can be written as

$$\frac{\partial C}{\partial \tau} + Pe\psi \frac{\partial C}{\partial \eta} = \frac{\partial^2 C}{\partial \eta^2} + \frac{1}{\zeta} \frac{\partial}{\partial \zeta} \left(\zeta \frac{\partial C}{\partial \zeta} \right), \tag{2.7a}$$

$$C(0,\eta,\zeta) = \delta(\eta), \tag{2.7b}$$

$$\frac{\partial C(\tau,\eta,1)}{\partial \zeta} = -\beta C(\tau,\eta,1), \quad \frac{\partial C(\tau,\eta,0)}{\partial \zeta} = 0, \quad (2.7c)$$

$$C(\tau, \pm \infty, \zeta) = \mathbf{0}. \tag{2.7d}$$

The *p*-th order concentration moments for scalar transport in flows are defined following the method proposed by Aris [36] as

$$C_p(\tau,\zeta) \equiv \int_{-\infty}^{+\infty} \eta^p C(\tau,\eta,\zeta) \mathrm{d}\eta.$$
(2.8)

Due to the characteristic of an exponential decay in space, distribution of the concentration is subjected to the auxiliary relations [36,12] as

$$\eta^{p}C(\tau,\pm\infty,\zeta) = \frac{\partial C(\tau,\pm\infty,\zeta)}{\partial \eta} = \eta^{p} \frac{\partial^{p}C(\tau,\pm\infty,\zeta)}{\partial \eta^{p}} = 0, \quad (p = 0, 1, 2, \cdots).$$

$$(2.9)$$

Applying the definition (2.8) to (2.7) with the aid of (2.9), we have

$$\frac{\partial C_p}{\partial \tau} = \frac{1}{\zeta} \frac{\partial}{\partial \zeta} \left(\zeta \frac{\partial C_p}{\partial \zeta} \right) + Pe\psi pC_{p-1} + p(p-1)C_{p-2}, \tag{2.10a}$$

$$C_p(0,\zeta) = C_{p0}(\zeta),$$
 (2.10b)

$$\frac{\partial C_p(\tau, 1)}{\partial \zeta} = -\beta C_p(\tau, 1), \quad \frac{\partial C_p(\tau, 0)}{\partial \zeta} = 0.$$
(2.10c)

Focused on the mean concentration distribution, the method of Aris's moments [36] is applied in the present work, in which the transverse averaged *p*-th order moment is given as

$$M_p(\tau) = \int_0^1 2\zeta C_p(\tau,\zeta) \mathrm{d}\zeta, \qquad (2.11)$$

and the averaged and normalized p-th central moments are devised as

$$\mu_p(\tau) = \frac{\int_0^1 \int_{-\infty}^{+\infty} 2\zeta (\eta - \mu_g)^p C d\eta d\zeta}{\int_0^1 \int_{-\infty}^{+\infty} 2\zeta C d\eta d\zeta},$$
(2.12)

where

$$\mu_{g}(\tau) = \frac{\int_{0}^{1} \int_{-\infty}^{+\infty} 2\zeta \eta C d\eta d\zeta}{\int_{0}^{1} \int_{-\infty}^{+\infty} 2\zeta C d\eta d\zeta} = \frac{M_{1}}{M_{0}}$$
(2.13)

is the longitudinal centroid of the mean concentration. The expressions for averaged central moments at higher orders in (2.12) give [31]

$$\mu_2(\tau) = \frac{M_2}{M_0} - \mu_g^2, \tag{2.14a}$$

$$\mu_3(\tau) = \frac{M_3}{M_0} - 3\mu_g \mu_2 - \mu_g^3, \qquad (2.14b)$$

$$\mu_4(\tau) = \frac{M_4}{M_0} - 4\mu_g\mu_3 - 6\mu_g^2\mu_2 - \mu_g^4.$$
(2.14c)

3. Exchange rate

The equation for the zero-th order concentration moment is corresponding to p = 0 in (2.10) as

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