



Transverse concentration distribution in Taylor dispersion: Gill's method of series expansion supported by concentration moments



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ABSTRACT

Presented in this paper is an analytical study of initial transition of the transverse concentration distribution in Taylor dispersion in a laminar tube flow. Gill's method of series expansion originally for the solution of the cross-sectional mean concentration is rigorously developed to obtain the transverse concentration distribution. Existing result by homogenization technique is analytically recovered as the special asymptotic expression of the finding by the present series expansion. With the mean concentration given by a Hermite polynomial based on the first four concentration moments to fully reflect the skewness and kurtosis, fourth-order series expansions are performed with sound convergence to detail the initial transition of the transverse distribution. Due to the velocity non-uniformity, the distribution of the transverse concentration in the central cross-section of the cloud appears as a "saddle" and attenuates gradually with the contribution of diffusion but does not disappear even at large time. The transition in transverse distribution is confirmed as one order of magnitude slower than that to longitudinal normality.

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1. Introduction

The concept of Taylor dispersion refers to the process that solute transports in flowing solvent under the combined effect of molecular diffusion and transverse non-uniformity of velocity [1]. The long term evolution of the cross-sectional mean concentration can be well described by a diffusion-like model. A virtual diffusivity, referred to as the Taylor dispersivity, to characterize this enhanced spread is in magnitude several orders larger than the molecular diffusivity. The associated Taylor dispersion model has been extensively applied in various areas such as environmental protection [2–9], chemical engineering [10], and energy exploitation [11].

Regarding to the mean concentration distribution, Aris [12] presented the method of concentration moments and obtained the first-moment and the asymptotic expression of the second moment. Gill [13] and Gill and Sankarasubramanian [14] proposed a generalized dispersion model of the mean concentration by a series expansion, and the same asymptotic dispersivity was obtained as that in [12]. The perturbation analysis of dispersion in a channel

flow with boundary reaction was presented in [3,15], among other efforts paid in this regard [16–18].

In Taylor's classical analysis [1], the dispersion model is supposed to apply after a period about $0.1a^2/D$ (a is the tube radius and D is the molecular diffusivity), characterized by the first root of the Bessel function of zeroth order. In context of the dispersion mechanism, naturally raised was the concern about the approach to the normality of mean concentration as an initial stage. Chatwin [19] proposed an asymptotic series expansion of concentration, and qualitatively outlined the occurrence and evolution of the skewness of the mean concentration distribution. According to Chatwin, the mean concentration reaches normality at the time scale of $1.0a^2/D$. Subsequently by extension of Aris' method of concentration moments, the third and fourth order moments indicating the skewness and kurtosis were obtained by the method of separation of variables [20,21], and the same time scale of the initial stage could be approximately obtained from corresponding Hermite polynomials.

In spite of all the efforts made to address the mean concentration distribution, the more difficult issue of equal importance about the transverse concentration distribution remained to be explored. For many applications, such as in environmental flows [6,9], solute transport under the effect of wall reaction [15,22–25], and risk assessment in groundwater and rivers [26–28], transverse peak concentration in the concentration cloud can be much

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higher than the transverse mean in the initial transition stage [29], and the usual estimate based on mean concentration does not work for a reliable assessment.

While molecular diffusion tends to smear out the variation towards transverse concentration uniformity, the concentration cloud is stretched by velocity non-uniformity to generate transverse concentration variation. The transition in transverse distribution has been preliminarily explored in [29] by a generalization of Mei’s homogenization technique [30,31]. As an essential conclusion, a time scale of $10a^2/D$ has been proposed to characterize the transition in transverse distribution. However, as common to all approximate techniques, both the analytical consistency of the solution to the basic well-posed mathematical model and the numerical accuracy of the solution need to be further validated and improved.

Provided in this work is an alternative analytical exploration of the evolution of transverse concentration distribution. Gill’s series expansion originally performed within second order for the solution of the mean concentration [13,14] is rigorously developed to the fourth order for the solution of the transverse concentration distribution. The mean concentration is taken as the Hermite polynomials based on the first four concentration moments to fully reflect the skewness and kurtosis of the mean concentration profile.

The specific objectives of this paper are: (I) to present the analytical model of the transverse concentration distribution by an extension of Gill’s series expansion up to fourth order; (II) to illustrate the analytical consistency between the present solution by series expansion and the previous one by homogenization and to test the convergence of the series expansion based on the first four concentration moments; and (III) to describe and characterize the transition in the transverse concentration distribution.

2. Formulation

2.1. Scalar transport

The scalar transport process in a fully developed steady laminar flow in a tube with radius a is governed by the advection–diffusion equation as

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} + D \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right), \quad (2.1)$$

where C is the concentration, t the time, u the flow velocity depending on the radial coordinate r , 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 $x = 0$ as

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

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

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

$$C(t, \pm\infty, r) = 0. \quad (2.3)$$

The non-penetration condition at the tube wall and symmetrical condition at the central axis read as

$$\frac{\partial C(t, x, 0)}{\partial r} = \frac{\partial C(t, x, a)}{\partial r} = 0. \quad (2.4)$$

With dimensionless variables introduced as

$$\tau = \frac{Dt}{a^2}, \quad \eta = \frac{x}{a}, \quad \zeta = \frac{r}{a}, \quad \Omega = \frac{\pi a^3}{Q} C, \quad Pe = \frac{\langle u \rangle a}{D}, \quad \psi = 2(1 - \zeta^2), \quad (2.5)$$

where $\langle u \rangle$ is the cross-sectional mean velocity, with the angle bracket indicating the operation of transverse average for a variable Q defined as

$$\langle Q \rangle \equiv \int_0^1 2\zeta Q d\zeta, \quad (2.6)$$

Then the governing equation and the initial and boundary conditions are rewritten as

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

$$\Omega(0, \eta, \zeta) = \delta(\eta), \quad (2.7b)$$

$$\Omega(\tau, \pm\infty, \zeta) = 0, \quad (2.7c)$$

$$\frac{\partial \Omega(\tau, \eta, 0)}{\partial \zeta} = \frac{\partial \Omega(\tau, \eta, 1)}{\partial \zeta} = 0. \quad (2.7d)$$

2.2. Extension of Gill’s series expansion

As a classical method, Gill’s series expansion [13,14] up to its second order has been extensively applied to exploring the longitudinal mean concentration distribution [32–34], however, the potential of this method to pursue the transverse concentration distribution has not been recognized previously.

Originally, Gill’s method is based on the generalized dispersion model as

$$\frac{\partial \langle \Omega \rangle}{\partial \tau} = \sum_{i=1}^{\infty} K_i(\tau) \frac{\partial^i \langle \Omega \rangle}{\partial \eta^i}. \quad (2.8)$$

By manipulation of (2.7) and its operation of transverse average with the introduction of the generalized dispersion model, we have corresponding series expansion for the transverse concentration distribution of

$$\Omega = \langle \Omega \rangle + \sum_{k=1}^{\infty} f_k(\tau, \zeta) \frac{\partial^k \langle \Omega \rangle}{\partial \eta^k}, \quad (2.9)$$

and for the transverse distribution functions $f_k(\tau, \zeta)$ an infinite set of differential equations is generated by comparing the coefficients of $\frac{\partial^p \langle \Omega \rangle}{\partial \eta^p}$ as

$$\frac{\partial f_1}{\partial \tau} = \frac{1}{\zeta} \frac{\partial}{\partial \zeta} \left(\zeta \frac{\partial f_1}{\partial \zeta} \right) - [Pe\psi + K_1(\tau)], \quad (2.10a)$$

$$\frac{\partial f_2}{\partial \tau} = \frac{1}{\zeta} \frac{\partial}{\partial \zeta} \left(\zeta \frac{\partial f_2}{\partial \zeta} \right) - [Pe\psi + K_1(\tau)]f_1 + [1 - K_2(\tau)], \quad (2.10b)$$

$$\begin{aligned} \frac{\partial f_{k+2}}{\partial \tau} = & \frac{1}{\zeta} \frac{\partial}{\partial \zeta} \left(\zeta \frac{\partial f_{k+2}}{\partial \zeta} \right) - [Pe\psi + K_1(\tau)]f_{k+1} + [1 - K_2(\tau)]f_k \\ & - \sum_{i=3}^{k+2} K_i(\tau) f_{k+2-i} \quad (k = 1, 2, \dots). \end{aligned} \quad (2.10c)$$

The initial and boundary conditions on f_k are given with the aid of (2.7b) and (2.7d) as

$$f_k(0, \zeta) = 0, \quad (2.11a)$$

$$\frac{\partial f_k(\tau, 0)}{\partial \zeta} = \frac{\partial f_k(\tau, 1)}{\partial \zeta} = 0. \quad (2.11b)$$

The transverse average operation of Ω gives

$$\int_0^1 \zeta f_k(\tau, \zeta) d\zeta = 0. \quad (2.12)$$

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