Axial diffusion effect on concentration dispersion

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ABSTRACT

This work presents an analytical attempt to illustrate the effect of axial diffusion on concentration dispersion in packed tube flows. The concentration moment method is applied to derive the analytical solution for time-dependent Taylor dispersion coefficient. With the increase in the packing parameter α as a damping factor, the concentration dispersion is characterized by three modes: (I) the shear-induced dispersion dominated mode, with dispersion coefficient determined by α; (II) the transition mode; and (III) the diffusion dominated mode, with dispersion coefficient determined by Péclet number Pe. In contrast to the usually negligible effects of axial diffusion for dispersion in pure fluid flows even at a relatively small Pe, axial diffusion with typical α plays an important role for packed media flows even with large Pe.

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1. Introduction

Concentration transport in packed media flows is of fundamental importance for its essential implications in various industrial and environmental processes, such as chromatography, biochemical separation or purification of mixtures, enhanced oil recovery, wastewater treatment engineering, and environmental risk assessment [1–11].

Among related studies on concentration transport in tube flows, Taylor's dispersion analysis provided a fundamental physical insight in characterizing the transverse mean concentration. Taylor dispersion [12] refers to concentration transport in tube flows under the effects of flow shear and molecular diffusion, which together contribute to a one-dimensional diffusion-like process. Usually the contribution of the flow shear effects dominates the process, and the effective diffusion coefficient, or Taylor dispersion coefficient, can be several orders of magnitude larger than the molecular diffusivity [1,13]. This predominant feature has attracted intensive studies and founded extensive applications [1,4,14–19].

Taylor dispersion in packed tube flows has been studied analytically [20,21]. Taylor's classical analysis and the homogenization technique were respectively applied for the dispersion coefficients.

However, these techniques belong to the asymptotic analysis and the analytical expressions obtained are only valid for dispersion at large times. In contrast, the concentration moment method first by Aris [22] is frequently adopted in the study of Taylor dispersion for its ability in capturing the temporal variation of the dispersion coefficient during the initial stage of the concentration transport, even when the flow is steady. Since the moment equations can be solved exactly, concentration moments at different orders contain accurate information on the evolution of the concentration cloud statistically. For example, the zeroth order moment reveals the conservation of the released mass; the first order moment reveals the effective displacement of the concentration cloud; the second order moment reveals the property associated with the dispersion of the concentration cloud. By obtaining the first three aforementioned moments, the transverse mean moments more exactly, it is capable of describing the concentration transport process with the aid of the Taylor dispersion model.

In Taylor's original study [12], the axial diffusion was neglected since the main focus of his analysis is on the notable enhancement of the solute dispersion by the flow distribution non-uniformity. A great deal of explorations by different methods extended Taylor's results to involve the axial diffusion effects in the dispersion coefficient [1,14,21–25], while at the same time indicated a quadratic Pe dependence for the enhancement of the dispersion, where the Péclet number Pe is a dimensionless parameter revealing the relative importance of the convection and diffusion, usually with large values for natural and industrial processes [1,26]. As a result the axial diffusion effects generally appear as an independent term in

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the analytical solutions for the dispersion coefficient, and are often neglected in related studies that followed.

Though a great deal of research has been undertaken on dispersion in packed media flows [7–9,20,21,27], there is no analytical study systematically addressed the effects of axial diffusion. Actually for the packed media, the dispersion process is much more complicated than that in pure fluid tube flows [21]. The axial diffusion can become important due to the packing of the media and in the transient initial stage of concentration transport. It is the flow details that strongly affect the concentration dispersion processes: the packed media in the tube reduce the transverse flow velocity non-uniformity, resulting in the decrease of the enhancement of the dispersion (or the shear-induced dispersion). That's the possible reason for axial diffusion playing an important role. On the other hand, the dispersion coefficient is numerically smaller at the transient initial stage of the transport while the effects of axial diffusion are not dependent on time, which also contributes to a more important contribution of axial diffusion to the dispersion process.

By the general formulation for concentration transport in packed media flows based on the phase average, Taylor dispersion and the effects of axial diffusion are analytically studied and discussed for packed tube flows in this paper. In Section 2, the analytical solution for Taylor dispersion coefficient is obtained by concentration moment method; and in Section 3, typical values of the packing parameter α as a damping factor are estimated, and three modes of the concentration dispersion as well as the transient initial stage on the effects of axial diffusion are discussed in detail.

2. Taylor dispersion in a packed tube flow

2.1. Formulation for concentration transport

The effects of diffusion and the transverse non-uniformity of longitudinal fluid flow velocity together contributes to the concentration transport. After an instantaneous release of concentration over the cross-section of a tube with pure fluid flow, the temporal evolution of the concentration cloud can generally be divided into two stages. The first stage can be called the transient initial stage of the transport, during which the transverse mean concentration shows a skewed longitudinal distribution. After a time scale characterized by R^2/D^*, where R is the tube radius and D^* is the molecular diffusivity, the mean concentration tends to a Gaussian distribution. At the latter stage, the centroid of the concentration cloud moves at the mean velocity of the flow, and the mean concentration disperses in the longitudinal direction by a virtual diffusion coefficient called Taylor dispersion coefficient [21,23,28].

For the more complicated case of a packed media flow, the basic equation for superficial concentration transport can be adopted generally at the phase average scale as [29]

$$\phi \frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{U}C) = \nabla \cdot (\kappa \lambda \phi \nabla C) + \kappa \nabla \cdot (\mathbf{K} \cdot \nabla C), \tag{1}$$

where $\mathbf{U}$ is velocity [m s^{-1}], t time [s], ϕ porosity [dimensionless], κ tortuosity [dimensionless] to account for the spatial structure of packed media, C concentration [kg m^{-3}], λ concentration diffusivity [m^2 s^{-1}], and $\mathbf{K}$ concentration dispersivity tensor [m^2 s^{-1}]. As diffusivity for concentration transport valid for the description of the single phase flow at the microscopic passage scale, concentration dispersivity is the property valid for the description of the effective flow at the phase average scale. By the operation of phase average, the discontinuity between the two phases of the ambient water and the solid packed material is smeared out. The equation is a combi-

nation of an advection–diffusion equation and a concentration dispersion law.

For the present case of a tube flow, Eq. (1) becomes

$$\frac{\partial C}{\partial t} + \frac{u}{\phi}\frac{\partial C}{\partial x} = \kappa\left(\lambda + \frac{K}{\phi}\right)\frac{\partial^2 C}{\partial x^2} + \kappa\left(\lambda + \frac{K}{\phi}\right)\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right). \tag{2}$$

Consider a uniform and instantaneous release of scalar substance with mass Q at the cross-section of $x = 0$ at time $t = 0$, the initial condition can be set as

$$C(x, r, t)|_{t=0} = \frac{Q\delta(x)}{\phi\pi R^2}, \tag{3}$$

where $\delta(x)$ is the Dirac delta function. The non-penetration condition at the tube wall of $r = R$ reads as

$$\left.\frac{\partial C}{\partial r}\right|_{r=R} = 0. \tag{4}$$

Since the amount of released substance is finite, we have upstream and downstream boundary conditions as

$$C(x, r, t)|_{x=\pm\infty} = 0. \tag{5}$$

With dimensionless parameters of

$$\tau = t \Bigg/ \frac{R^2}{\kappa\left(\lambda + \frac{K}{\phi}\right)}, \quad \xi = x \Bigg/ \frac{R^2 u_m}{\kappa(\phi\lambda + K)} - \tau,$$

$$\zeta = \frac{r}{R}, \quad \Omega = C \Bigg/ \frac{Q}{\phi\pi R^2}, \tag{6}$$

where u_m is the transverse mean velocity, the governing equation and its initial and boundary conditions for the concentration transport can be rewritten as

$$\frac{\partial\Omega}{\partial\tau} + \psi'\frac{\partial\Omega}{\partial\xi} = \frac{1}{\mathrm{Pe}^2}\frac{\partial^2\Omega}{\partial\xi^2} + \frac{1}{\zeta}\frac{\partial}{\partial\zeta}\left(\zeta\frac{\partial\Omega}{\partial\zeta}\right), \tag{7}$$

$$\Omega(\xi, \zeta, \tau)|_{\tau=0} = \delta(\mathrm{Pe}\,R\xi), \tag{8}$$

$$\left.\frac{\partial\Omega(\xi, \zeta, \tau)}{\partial\zeta}\right|_{\zeta=1} = 0, \tag{9}$$

$$\Omega(\xi, \zeta, \tau)|_{\xi=\pm\infty} = 0, \tag{10}$$

where

$$\psi' = \frac{u}{u_m} - 1 \tag{11}$$

and

$$\mathrm{Pe} = \frac{Ru_m}{\kappa(\phi\lambda + K)} \tag{12}$$

is the Péclet number for concentration transport in packed tube flows.

2.2. Concentration moment method and analytical solution for dispersion coefficient

The pth order concentration moment is defined as

$$m_p(\zeta, \tau) = \int_{-\infty}^{+\infty} \xi^p \Omega(\xi, \zeta, \tau) d\xi. \tag{13}$$

Characteristic of an exponential decay in space, distribution of the concentration is subjected to the auxiliary relations [22,23] as

$$\xi^p\Omega(\xi, \zeta, \tau)|_{\xi=\pm\infty} = \left.\frac{\partial\Omega(\xi, \zeta, \tau)}{\partial\xi}\right|_{\xi=\pm\infty} = \xi^p\left.\frac{\partial^p\Omega(\xi, \zeta, \tau)}{\partial\xi^p}\right|_{\xi=\pm\infty} = 0$$

$$(p = 1, 2\ldots). \tag{14}$$

Multiplying Eqs. (7)–(9) by ξ^p and integrating them with respect to ξ in the interval of $(-\infty, \infty)$ with the aid of Eqs. (10) and (14), we have