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Complete spatial concentration distribution for Taylor dispersion in packed tube flow

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ABSTRACT

Understanding solute transport process is of fundamental significance for industrial and natural processes such as mixing and separation. Since detailed information for the transverse concentration distribution is required for associated applications, compared with the sole consideration of the cross-sectional mean concentration in previous studies, the present paper analytically explores the complete spatial concentration distribution in packed tube flow by the proposed two-scale perturbation analysis (Z. Wu, G.Q. Chen, Journal of Fluid Mechanics, 740 (2014) 196–213.). With modification on the zeroth-order concentration up to the first-order, the deduced analytical solution gives a good prediction for the longitudinal distribution of mean concentration as well as the transverse distribution, according to comparisons with new results of numerical simulation. Importantly we show in the paper that instead of being uniformly distributed in the cross-section as expected in traditional view, the transverse concentration is highly non-uniform when Taylor dispersion model is applicable. Representing the complicated flow conditions for packed tube flow, the unique dimensionless parameter as a damping factor affects the complete spatial concentration distribution in two ways: cause the contraction of the solute concentration cloud, and the flattening of the concentration contours.

1. Introduction

Understanding solute transport process is of great importance for various applications in different fields. For industrial or environmental processes such as mixing and separation [1–3], pollution control [4,5], ecological restoration and wastewater treatment engineering associated with wetlands [6–10], knowledge for the concentration distribution and evolution is primarily concerned [11–14]. And among the associated configurations, solute transport in packed media flow, or packed tube flow as studied in this paper, is a most typical one.

Taylor dispersion [15] describes an asymptotic stage of the concentration transport with the cross-sectional mean concentration governed by a "diffusion process" in the flow direction. The concept is so interesting and important that it has been intensively studied and extensively applied in different fields in the past few decades [2,16–21]. It is well know that if the flow velocity is uniform across the cross-section of the tube, the solute transport process follows a diffusion equation at a longitudinally moving coordinate with a speed of the fluid flow. However, Taylor [15] pointed out that even though there is a transverse distribution for the flow velocity (non-uniform), after a given initial stage the solute transport can also be described by a diffusion equation, although with a much greater "diffusivity" than the molecular diffusivity; and the centroid of the solute cloud longitudinally moves at a constant speed, too, which turns out to be the cross-sectional mean velocity of the flow. For the mechanism, the non-uniformity of transverse distribution of the flow velocity and the transverse molecular diffusion together contribute to this "enhanced diffusion", usually leading to a several orders of magnitude greater "diffusivity" in practical applications [22,23].

Solute transport in packed tube flow is much more complicated than that in pure fluid flow [24,25]. And a great deal of research works have been carried out at different angles in recent years. For example, there are studies focusing on the detailed pore-scale flow and transport processes, mainly based on the massive computational efforts [26,27]. To analytically tackle the problem, Professor Chen and his group explored Taylor dispersion process at the holistic scale, on the basis of phase average [24,25,28–30]. The operation of phase average is to smear out the discontinuity caused by the irregular solid packed media in

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the considered region, resulting in a continuous distribution for both the velocity and concentration at the phase-average scale. Thus the analysis for pure fluid flow can be extended to study solute transport in packed media flow. In this paper, we perform the study under this established framework.

The concept of Taylor dispersion is traditionally applied for the cross-sectional mean concentration [5,10,23,29,31]. In previous efforts for solute transport in packed tube flow, different analytical approaches were applied for the mean concentration distribution, either for a single-zone tube with homogeneous media packed in [24] or for a two-zone configuration with heterogeneity of media distribution [25]. However, in some environmental or industrial processes we need not only the longitudinal mean concentration, but also the transverse concentration distribution details. In a recent progress, Wu and Chen [23,32] have shown that the transverse concentration distribution difference can be remarkable for a very long period after Taylor dispersion model is valid for solute transport in pure fluid flow, indicating the great significance of exploring the detailed transverse concentration distribution patterns.

To study the complete spatial concentration distribution for Taylor dispersion process, the traditional one-dimensional Taylor dispersion model is insufficient. As an extension based on the homogenization technique, the two-scale perturbation analysis proposed by Wu and Chen [23,32] provides an appropriate analytical approach for the present exploration. It is shown that by introducing the longitudinal correction functions and considering the higher-order perturbation problems other than that up to the second-order, the deduced analytical solution captures the longitudinal skewness of the concentration distribution, which is important in constructing the complete spatial concentration distribution.

In this paper, we adopt the two-scale perturbation analysis to study the complete spatial concentration distribution for solute transport in packed tube flow at the phase-average scale. The article is structured as follows. In Section 2, we give the formulation illustrating the configuration, the governing equations, and the perturbation problems. In Section 3, the analytical solution with modification on the zeroth-order concentration up to the first-order is deduced. Section 4 provides a simple numerical validation for the obtained analytical solution, and further discussions. Conclusions are given at the end of the paper.

2. Formulation

Solute transport process in packed tube flow is of great complexity for the existence of the irregular packed media in the concerned region, which causes the discontinuity of flow and concentration in space, and the complicated additional boundary conditions at the surface of the packed media changing the local flow and concentration distributions. Instead of studying the process at the pore-scale characterized by the typical transverse scale of the flow path, we explore the problem at an intermediate phase-average scale, applying the phase average operation to smear out the discontinuity [25,33,34]. Since the resulted flow and concentration distribution is continuous, the analysis we applied for the pure fluid flow can thus be directly extended for the present study.

The previous analytical explorations for solute transport have mainly focused on the longitudinal distribution of mean concentration, and only some limited research work discussed the transverse distribution, such as the one by Bolster et al. [35]. In the reference, the authors applied a volume averaging approach to calculate the concentration distribution, although their primary concern is to quantify mixing by the acquired information. Actually, the volume averaging and the homogenization (which is the basis of the present research) techniques have much in common, for example, they both need to determine the "closure problems" at the "micro-scale" fields, the information of which is required for the macro-scale descriptions of the process (such as the effective coefficient in Taylor dispersion model). However, to reveal the transverse concentration distribution details, the "micro-scale" fields are much more emphasized.

The governing equation for concentration transport in packed media flow at the phase-average scale is adopted as [25,33,34]

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

where ϕ is porosity, C concentration, t time, $\mathbf{U}$ superficial velocity, κ tortuosity, λ concentration diffusivity, and $\mathbf{K}$ concentration dispersivity tensor.

The radius of the packed tube is R. In a Cylindrical coordinate system, x-axis aligns with the longitudinal direction, r-axis the radial direction, and O at the central line of the tube is the origin. For the idealized case of homogeneous packed tube with constant physical parameters ϕ, κ, λ, and K, Eq. (1) is simplified into

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

where the superficial velocity u is only a function of the radial coordinate r.

For a pulsed injection of the solute across the plane $x=0$, the initial and boundary conditions are respectively given as

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

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

and

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

where Q is the released mass and $\delta(\cdot)$ the Dirac delta function.

For the perturbation problems by the two-scale perturbation analysis [23,32], we first define the transverse-average operation for any given quantity v as

$$\langle v\rangle\equiv\int_0^1 2\zeta\, v\,\mathrm{d}\zeta. \tag{6}$$

Introducing the following dimensionless parameters:

$$\psi=\frac{u}{\langle u\rangle},\quad \tau=t\Big/\frac{\phi L}{\langle u\rangle},\quad \xi=\frac{x}{L}-\tau,\quad \zeta=\frac{r}{R},\quad \epsilon=\frac{R}{L},$$
$$\mathrm{Pe}=\frac{\langle u\rangle R}{\phi\kappa\left(\lambda+\frac{K}{\phi}\right)},\quad \Omega=C\Big/\frac{Q}{\phi\pi R^2}, \tag{7}$$

with L is a longitudinal characteristic length, the governing equation Eq. (2) can be rewritten as

$$\epsilon\frac{\partial\Omega}{\partial\tau}+\epsilon\psi'\frac{\partial\Omega}{\partial\xi}=\epsilon^2\frac{1}{\mathrm{Pe}}\frac{\partial^2\Omega}{\partial\xi^2}+\frac{1}{\mathrm{Pe}}\frac{1}{\zeta}\frac{\partial}{\partial\zeta}\left(\zeta\frac{\partial\Omega}{\partial\zeta}\right). \tag{8}$$

Here

$$\psi'\equiv\psi-\langle\psi\rangle \tag{9}$$

defines the velocity deviation, and the prime can represent the deviation of any quantity from its mean. In Eq. (8), ψ' is introduced by the adoption of the longitudinally moving coordinate system with the transverse mean velocity of the flow: mathematically, the moving system is expressed by the definition of the longitudinal variable

$$\xi=\frac{x}{L}-\tau, \tag{10}$$