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NUMERICAL SIMULATION OF THE DISPERSION IN OSCILLATING FLOWS WITH REVERSIBLE AND IRREVERSIBLE WALL REACTIONS*

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Abstract: This is a study on the mass transport of a solute or contaminant in oscillating flows through a circular tube with a reactive wall layer. The reaction consists of a reversible component due to phase exchange between the flowing fluid and the wall layer, and an irreversible component due to absorption into the wall. The short-time dispersion characteristics are numerically investigated, incorporating the coupling effects between the flow oscillation, sorption kinetics, and retardation due to phase partitioning. The effects of various dimensionless parameters e.g., Da (the Damköhler number), α (phase partitioning number), Γ (dimensionless absorption number), and δ (dimensionless Stokes boundary layer number) on dispersion are discussed. In particular, it is found that there exist trinal peaks of the breakthrough curves in some cases.

Key words: dispersion, flow oscillation, wall reactions

1. Introduction

This work aims to investigate, through numerical simulations, the behaviour of the short-time dispersion in oscillatory flow through a straight circular tube, whose wall is lined with a thin layer in which the solute may undergo reversible and irreversible chemical reactions. The long-time dispersion of a substance in a laminar fluid flow through a long tube was first analyzed theoretically by Taylor[1] who obtained an analytical solution for the sectionally-averaged concentration. Later, Aris[2], Elder[3] and Mayock et al.[4] among many others, were all mainly devoted to finding the long-time steady behaviour of the dispersion theoretically. So far, the fully developed dispersion without flow oscillation and wall reactions has been a relatively well-understood process. Meanwhile there have been a few researches that take into account both flow oscillation and chemical reactions on the wall. For example, Liu[5], Liu and Cai[6] extended Taylor's dispersion theory to two-dimensional unsteady flows, Mazumder and Das[7], Jiang and Grotberg[8], Liu[9,10] studied the effect of wall absorption on axial dispersion in oscillatory tube flow. Davidson and Schroter[11]and Phillips and Kaye[12] studied a reversible phase exchange reaction. Very recently Ng[13-17] studied theoretically the long-time asymptotic

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state of the dispersion in a tube flow, incorporating the coupling effects between the flow oscillation, sorption kinetics, and retardation due to phase partitioning. Research interest of the dispersion in more complex and practical problems such as pollutant dispersion in urban areas[18], electrophoretic separation of a mixture of chemical species[19] and dispersion of dissolved species and suspended particles in marsh and wetland systems[20] is increasing in the last decade.

Of equal practical interest is the initial transient dispersion of a mass cloud, which deserves attentions for many reasons. The short-time dispersion is important, for examples, in the following areas: (1) many tubes (e.g., human arteries and airways) are so short that the travelling time along the tube may not be long enough for the large-time dispersion behaviour to appear, (2) the concentration distribution is highly skewed and non-Gaussian during the early phases of transport, and the breakthrough curves may exhibit double peaks, this kind of behaviour can have non-trivial implications to chromatographic separation (e.g., Refs.[21,22]), and (3) the long-time transport equation requires an initial condition that depends on the early transient development (e.g., Ref.[23]). However, the investigation of transient early-stage dispersion taking the flow oscillation and wall chemical reactions into account is quite limited except in the above-mentined articles and the references therein. The main objective of this study is to find out how oscillation and chemical reactions affect the transient transport behaviour in a straight circular tube.

The article is organized as follows. In the next section, the governing equations and numerical method are described, with inclusion of the introduction to the LCPFCT algorithm and its implementation. In Section 3, the behaviour of the short-time dispersion in an oscillatory flow with wall reaction is simulated. The evolution curves of the centre and variance of mass are plotted and compared, and the effects of wall reaction and oscillation on the sectional averaged concentration are discussed. The conclusions are drawn in Section 4.

2. Governing equations and numerical method

The dispersion of a cloud of a chemical species (e.g., contaminant), which is soluble in or miscible with the fluid in an oscillatory, circular tube flow, is governed by

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} + \tilde{u}\frac{\partial \tilde{c}}{\partial \tilde{z}} = D\left(\frac{\partial^2 \tilde{c}}{\partial \tilde{r}^2} + \frac{1}{\tilde{r}}\frac{\partial \tilde{c}}{\partial \tilde{r}}\right)$$

$$\text{in } -\infty < \tilde{z} < \infty,\ 0 < \tilde{r} < a \tag{1}$$

along with the boundary conditions

$$-D\frac{\partial \tilde{c}}{\partial \tilde{r}} - \tilde{\Gamma}\tilde{c} = \frac{\partial \tilde{c}_s}{\partial \tilde{t}} = k(\tilde{\alpha}\tilde{c} - \tilde{c}_s) \quad \text{at } \tilde{r} = a \tag{2}$$

$$\frac{\partial \tilde{c}}{\partial \tilde{r}} = 0 \quad \text{at } \tilde{r} = 0 \tag{3}$$

where $\tilde{c}(\tilde{z},\tilde{r},\tilde{t})$ is the fluid-phase concentration given by the mass of the mobile phase of the species dissolved per volume of fluid, while $\tilde{c}_s(\tilde{z},\tilde{t})$ is the wall-phase concentration given by the mass of the stationary or immobile phase retained per area of tube wall, $\tilde{t}$, $\tilde{r}$ and $\tilde{z}$ are the time, the radial coordinate and the axial coordinate respectively. We also denote the molecular diffusion coefficient by D, the irreversible absorption rate by $\tilde{\Gamma}$, the reversible phase exchange rate by k and the equilibrium partitioning ratio between the mobile and immobile phases by $\tilde{\alpha}$. In addition, the velocity $\tilde{u}$ driven by a given oscillatory pressure gradient is as follows:

$$\tilde{u}(\tilde{r},\tilde{t}) = \hat{u} + Re(u_{\tilde{\omega}}\mathrm{e}^{-\mathrm{i}\tilde{\omega}\tilde{t}}) \tag{4}$$

where

$$\hat{u} = \tilde{u}_0\left(1 - \frac{\tilde{r}^2}{a^2}\right) = K\frac{a^2}{4\nu}\left(1 - \frac{\tilde{r}^2}{a^2}\right) \tag{5}$$

is the steady component of the velocity, and

$$u_{\tilde{\omega}} = \mathrm{i}\frac{K\phi}{\tilde{\omega}}\left\{1 - \frac{J_0\left[\dfrac{(1+\mathrm{i})\tilde{r}}{\tilde{\delta}}\right]}{J_0\left[\dfrac{(1+\mathrm{i})a}{\tilde{\delta}}\right]}\right\} \tag{6}$$

is the complex amplitude of the oscillatory component of the fluid velocity. $\tilde{\omega}$ in Eqs.(4) and (6) is the angular frequency of the oscillation, ϕK in Eq.(6) is the amplitude of the oscillatory part of the pressure gradient, and $J_0(x)$ is the zeroth-order Bessel function of the first kind, $\tilde{\delta} = \sqrt{2\nu/\tilde{\omega}}$ is the thickness of the Stokes boundary layer resulting from the oscillation of the flow. Note that in Eq.(1) the axial diffusion term has been ignored due to its much less significance compared to the convective term.

By introducing the following normalized quantities