



Numerical study on mass transfer from a composite particle settling in a vertical channel



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ABSTRACT

A two-dimensional study of mass transfer from a circular composite particle settling in a vertical channel is conducted with the lattice Boltzmann method. The particle is composed of two materials, one insoluble while the other soluble in the ambient fluid. In the problem, mass transfer, particle motion and fluid flow are closely coupled, where the concentration at the particle surface and particle properties vary with mass transfer. It is observed that mass transfer follows a Schmidt number independent scaling law of $[t/(t_v\sqrt{Sc})]^{-1.5}$ (t is the physical time, t_v is the momentum diffusion time scale and Sc is the Schmidt number), which is quite different from the pure diffusion of a stationary particle, $\sim (t/t_x)^{-0.5}$ (t_x is the mass diffusion time scale). An analysis of the concentration and flow pattern around the particle suggests that the scaling law for a settling particle is related to both diffusion distance and convection distance, while it is only relevant to the diffusion distance in the case of a stationary particle. For a settling particle, mass transfer is enhanced by two mechanisms due to convection, i.e., the concentration around the particle surface transported to the downstream of the particle by the fluid flow and the interface of mass transfer stretched with the particle motion, which are absent in the case of a stationary particle. Thus, the rate of mass transfer in the case of a settling particle is much higher than that for a stationary particle.

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1. Introduction

Due to its broad existence in industrial and natural processes, such as fluidized beds, lubricated transport, fluvial erosion, river sediment and sand storms [1,2], understanding the mechanisms of the transport of solid particles in a fluid is of great significance. In the past decades, numerous works have been done in the field [3–11]. For example, Segré and Silberberg [3] conducted an experimental study on the motion of particles in a pipe flow, and discovered that the neutrally buoyant particles always migrate to a certain lateral equilibrium position, which is the so-called Segré-Silberberg effect. Hu et al. [4] studied the two-dimensional sedimentation of a circular particle in a vertical channel with the finite-element method, and reported that the particle would drift to the centerline of the channel at small Reynolds numbers while it was off the centerline at higher Reynolds numbers. Feng et al. [5] investigated the sedimentation of a circular particle under different Reynolds numbers, and identified five regimes of motion. Cate et al. [8] studied a single sphere settling under gravity both experimentally and numerically, and found that the agreement between experiments and simulations was satisfactory.

In most of previous studies, the particles are inert, i.e., there is no mass transfer between particles and the fluid. Usually, in numerous industrial and natural processes, mass transfer from the particle surface to the surrounding fluid can occur, such as pollutant materials and pollen grains, and some studies on mass transfer between particles and the fluid have been reported [12–16]. For instance, Batchelor et al. [12] studied mass transfer across a suspended particle in the fluid with a steady linear velocity distribution, Feng et al. [13] examined the unsteady mass transfer process across a spheroid with small Peclet numbers, Subramanian et al. [14] studied the inertial effect on mass transfer across neutrally buoyant spheres in a steady linear velocity field, Yang et al. [15] investigated mass transfer across a neutrally buoyant sphere in a shear flow at finite Reynolds and Peclet numbers, and Zhang et al. [16] presented an investigation on mass transfer across a single sphere in a creeping flow.

The above studies, however, are based on two underlying assumptions, namely, the concentration at the particle surface is constant, and the particle properties do not vary with mass transfer. These two assumptions may be invalid in some cases, such as coal combustion, food processing, pharmaceutical industry and soil erosion [17–23], where particles are composed of different materials, some of which are insoluble while others are soluble in the ambient fluid. For such composite particles, the concentration

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at the particle surface can be related to the mass of soluble components inside the particle, i.e., the concentration at the particle surface can decrease with mass transfer. More importantly, the particle properties, such as density, mass and moment inertia, will vary with mass transfer, which influence the particle motion and fluid flow significantly, and mass transfer can then be affected in turn by the particle motion and fluid flow due to the convection effect. In early works [24–26], flows over multiple and non-spherical particles with mass transfer are studied, but the particles cannot move freely, where mass transfer and particle motion are decoupled artificially. In numerous industrial processes, such as pharmaceutical industry, the particles are transported by the fluid flow, where mass transfer and particle motion can affect each other. To our knowledge, studies on the transport of such composite particles with mass transfer are rarely reported in the literature, and the present work aims to deepen our understanding.

The rest of the present paper is organized as follows. Section 2 will describe the setup of the problem, in Section 3, we will briefly introduce the numerical method, and our code will be validated in Section 4. In Section 5, the two-dimensional results and discussions will be reported, and some conclusions will be drawn in Section 6.

2. Problem description

The setup of the problem is depicted in Fig. 1. Initially, a circular composite particle with diameter D_p is positioned at (x_0, y_0) in a vertical channel with width W and height H . Under the gravity acceleration g , the particle will settle down. Different from an inert particle, the particle is composed of two materials, one insoluble while the other soluble in the ambient fluid. The insoluble component is undeformable and forms the particle shell, while the soluble component distributes uniformly inside the particle.

With the soluble component dissolving in the ambient fluid, the rate of mass transfer across the particle surface can be expressed as [12]

$$\frac{dm_s}{dt} = - \oint_{\Gamma} \alpha \nabla C \cdot \mathbf{n} ds, \quad (1)$$

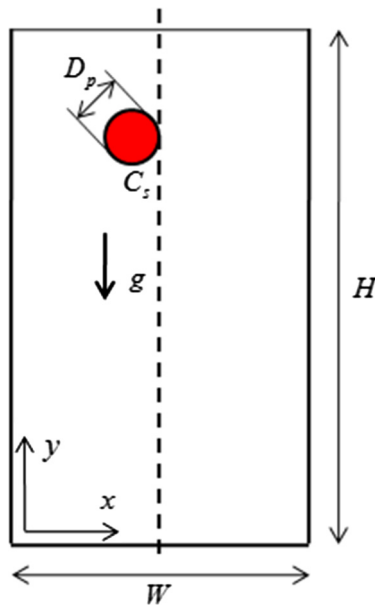


Fig. 1. Sketch of a circular composite particle with mass transfer settling in a vertical channel.

where m_s is the mass of the soluble component inside the particle, α is the mass diffusivity, ∇C is the concentration gradient of the soluble component around the particle surface, and \mathbf{n} is the unit vector normal to the particle surface. With mass transfer, the mass of the soluble component inside the particle will decrease. Since the soluble component distributes uniformly inside the particle, the concentration of the soluble component at the particle surface decreases as well. In previous studies [12–16], however, the concentration at the particle surface is set to be constant artificially, which cannot reflect the decreasing mass of the soluble component with mass transfer. In the present study, to build the relationship between the mass of the soluble component and the concentration at the particle surface, we assume the concentration of the soluble component at the particle surface C_s to be the mass ratio of the soluble component γ , i.e.,

$$C_s = \gamma = \frac{m_s(t)}{m_s(0)}, \quad (2)$$

where $m_s(0)$ is the initial mass of the soluble component inside the particle. It is clear that C_s varies in the range of $[0, 1]$, i.e., C_s is relatively high at the start, and decreases to zero with mass transfer of the soluble component.

With mass transfer from the particle to the fluid, the particle mass will vary with time. Initially, the particle mass is composed of two parts, i.e.,

$$m_p(0) = m_i + m_s(0), \quad (3)$$

where m_i is the mass of the insoluble component which is a constant. With the dissolution of the soluble component, the dissolved volume will be occupied by the ambient fluid, as a result, the particle mass will include three parts, i.e.,

$$m_p(t) = m_i + m_s(t) + m_f(t), \quad (4)$$

where $m_f(t)$ is the mass of the fluid diffusing into the particle to occupy the dissolved volume. Assuming that both the fluid and soluble component are incompressible, we have

$$m_f(t) = \rho_f \frac{m_s(0) - m_s(t)}{\rho_s}, \quad (5)$$

where ρ_f and ρ_s are the densities of the fluid and soluble component, respectively. We should point out that the permeability of the particle is assumed to be large enough, thus, the distribution of the fluid inside the particle is uniform. Since the insoluble component is undeformable, the particle shape and size are kept fixed, i.e., the particle diameter is constant, as a result, the particle density $\rho_p(t) = m_p(t)/A_p$ and moment inertia $I_p(t) = m_p(t)D_p^2/8$ will vary with mass transfer as well, where $A_p = \pi D_p^2/4$ is the particle area (since it is a two-dimensional study).

In the problem, three dimensionless numbers are involved, i.e., Peclet number $Pe = D_p U_p / \alpha$, Reynolds number $Re = D_p U_p / \nu$ and Schmidt number $Sc = \nu / \alpha$, where U_p is the velocity of the particle during sedimentation, ν is the kinematic viscosity of the fluid, and α is the mass diffusivity.

3. Numerical method

3.1. Lattice Boltzmann method

In the present study, the double-population lattice Boltzmann method for flows with the convection-diffusion process is adopted, in which the flow and concentration fields are solved respectively with two lattice Boltzmann equations (LBEs) [27],

$$f_i(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t) - f_i(\mathbf{x}, t) = \Omega_i(f), \quad (6)$$

$$g_i(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t) - g_i(\mathbf{x}, t) = \Omega_i(g), \quad (7)$$

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