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Mass transfer enhancement in non-Brownian particle suspension under a confined shear

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ABSTRACT

This paper shows the effect of the hydrodynamic interactions between non-Brownian isotropic particles for mass transfer enhancement in a shear flow generated by sliding walls in two dimensions through the direct numerical simulations. The particles are considered as a separate phase, while suspending solvent is modeled using the Stokes equation of which inertial and buoyancy effect are neglected. In the numerical simulation, we employ the finite element method to discretize the spatial domain with an explicit time stepping method. Interface capturing method is used to identify the boundary between the particle and the fluid. Automated adaptive mesh refinement is employed to increase the resolution in the vicinity of the particle boundaries as well as the interface between the solute and solvent. We investigate the effect of the particle hydrodynamics on mass transfer when the solute transports into the solvent and compare the mass transfer enhancements as a function of area fraction of multi-non-Brownian particles contributed. It is found that the mass transfer is enhanced by 3.6% in 1.0% area fraction which is a critical particle area fraction for the present flow conditions.

1. Introduction

The mass transfer of the solute into the solvent is significantly influenced by the presence of the particles and it depends upon the particle size, shape and so on. It is considered as a heterogeneous medium in which dispersed materials such as solid particles, droplets or bubbles are distributed in a continuous phase for the solute and the solvent. When the particles are suspended into the solvent, they generate the viscous resistive force against the solvent flow, referred as the hydrodynamic drag and also give rise to the interactions continuously to change the configuration of the suspended particles. This invokes the velocity disturbance around the particles and consequently the solute migrates into the solvent with the disturbed pattern on the mass transfer.

Many studies on the transportation of the gas–liquid phase in suspended solid particle residing in the interface layer of two phases have reported that the mass transfer is enhanced due to the particle contribution [1–4]. The positive effect of the particles was also observed for the enhancement of the absorption rate of oxygen into a liquid [5]. In the case of gas–liquid–liquid system, oil-in-water systems with a dispersed liquid phase, the research histories and underlying possible mechanisms for mass transfer enhancement with the effect of the contribution of dispersed phase were summarized in the review paper [6]. A few papers have been reported in the different theoretical approach with heterogeneous model [7–9] and the pseudo-homogeneous model for suggesting the theoretical mechanism on mass transfer enhancement in suspension [10]. These models were applied to the enhancement of the mass transfer rate for the gas absorption in the suspension of nano-size particles considering the Brownian motion [11]. Recently, the dispersion model was proposed to depict the mass diffusion enchantment in nanofluids in diluted fixed beds [12].

In the aspect of the numerical simulation, one of the major challenges in simulating the flow of a large number of suspended particles is the complex geometry of the flow domain, which is continually changing as the particles move relative to one another. A number of different approaches have been successfully developed, which can be roughly divided into two groups depending upon how the particle boundaries are treated. The first group is the method where the computational mesh is fitted to the boundaries of the particles, so that the computational domain consists only of fluid between the particles. The fluid–particle interface is partitioned into a finite set of pieces. This is termed an 'interface fitting method', and requires that the mesh is continuously deformed as the particles move such as an Arbitrary Lagrangian Eulerian method (ALE) [13] and a fully Lagrangian method [14]. These methods provide highly accurate solutions as the boundary conditions do not have to be interpolated onto the mesh, and the mesh is usually adapted to provide greater precision near the particle surfaces. They are

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relatively simple to implement if the mesh connectivity does not change but this will limit the particle motion to small-scale and simple behavior. However, for any significant particle motion, the mesh becomes distorted and consequently the accuracy of the solution can deteriorate. The second approach is to compute the flow within the entire suspension and to impose the conditions of rigid body motion on the parts of the domain corresponding to the rigid particles. This is termed an 'interface capturing method'. The interface is reconstructed from the properties of associated field variables. This can be achieved by introducing forcing terms at the positions of the particle boundaries such as in the fictitious domain method developed by Glowinski et al. [15]. Hwang and co-workers have successfully used this method to study sheared suspensions of particles in both Newtonian [16]. A major advantage of this approach is that the computational domain is usually simple and fixed, and so can be solved using a fixed grid independent of the positions of the particles. However, the price for this simplicity is that the grid resolution must be sufficiently fine throughout the whole computational domain to provide adequate resolution near the particle boundaries. In this paper, for the particle dynamics, we do not employ explicitly to track the surface of a particle, but a particle is regarded as a highly viscous fluid compared to that of a surrounding fluid and then tracked via the average velocity over the phase of a particle. This is also analogous to the method 'fluid particle dynamics (FPD)' employed in [17,18]. The major advantage of this method is that we can avoid tracking the surface of a particle providing with numerical difficulties in imposing the boundary condition. We also introduce automated mesh refinement (AMR) to refine the mesh in specific parts of the domain. The main aim of AMR is to increase the resolution in only certain areas of the spatial domain. We can thus ensure an accurate finite element solution at much lower computational cost compared to a fully refined mesh. For the particle suspension problem an increased resolution is especially required around the surface of particle, because we need to have a good approximation of the disturbance acting on the particle. Therefore, we prescribe a mesh around the particle surface that is highly refined compared to other areas of the domain. This enables us to minimize the phenomena of smearing out the information at the particle–fluid interface. Because the purpose of this study is to consider the mass transfer of the solute in suspending particles, we also consider the mesh adaptivity for the interface between the solute and the solvent corresponding to the refinement for surface of the particles consistently. Through this way, we are able to achieve the necessary resolution near the particle boundaries and the regions between the solute and solvent with a much smaller total number of degrees of freedom.

In this paper, we shall consider the interactions between the multi-isotropic particles suspending into the Newtonian fluid when the solute is convectively diffused into the solvent in the confined shear between parallel walls. The dispersed phase consists of circular solid particles, in effect, long cylinders that do not deform, but are free to translate and rotate. Therefore, we determine how the disturbance generated by the hydrodynamic interactions in the particle suspension affects the solute transfer into the solvent. We thus study how far the interface between the solute and the solvent is influenced by hydrodynamics of the circular solid particles on the mass transfer under confined shear by using the adaptive direct numerical simulations. This is implemented by comparison of mass transfer area fraction of the solute transferred into the solvent in both of the absence of particles and the presence of suspended particles and accordingly studied the effect of a function of area fraction of the particles on the mass transfer enhancement.

2. Mathematical model

Without any chemical reaction between the solute and solvent as the external force, we shall consider only the advection–diffusion problem so that the kinetics for the interface is not included. The convective force on the solute is primarily responsible for inducing the mass transfer to the solute so that the interfacial convection induced by the diffusion is neglected. The solute is weakly diffused relative to the convection. We shall assume that the length scales of the fluid flow are sufficiently small so that the viscous force can surpass the inertia and body forces as Kreiger assumed [19]. Hence, inertial and buoyancy effects are neglected. We also assume the length-scale of the suspending particles to be sufficiently large that each phase can be described by continuous field. Thus, the scale of the diffusion of suspended particles is enough small to the convection, which simplify to model the particle motion without taking into the account the thermal fluctuation such as a Brownian motion. This can deduce that the motion of particles in flow is purely corresponded along the streamlines formed by hydrodynamic interactions between particles. Our interest focuses on the disturbances around the surface of the particles solely generated by the particle–fluid interactions and accordingly the impact on the mass transfer.

For a computation domain to simulate the mass transfer system in suspended particles, we divide the volume Ω into the volume occupied by the solute phase Ω_s, solvent phase Ω_f and the collective regions occupied by the particle phase $\Omega_P = \cup_{i=1}^{n} \Omega_{P_i}$. The boundary around each suspended domain is denoted by Γ_{P_i}. The whole of the boundaries are denoted by $\Gamma = \Gamma_\Omega + \Gamma_{P_i}$. Fig. 1 shows the schematic diagram of the computational domain. Brownian motion may be neglected when the Peclet number (Pe_1) for the particle suspension defined by Eq. (1) approaches infinity, meaning that the advection of particles dominates the thermal fluctuations,

$$Pe_1 = \frac{\dot{\gamma} a^2}{D_f}, \tag{1}$$

where $\dot{\gamma}$ is the shear rate, a is the particle radius and D_f is the diffusivity for a sphere in a fluid. Since the flow is assumed to be incompressible, isothermal, inertialess and neutrally buoyant, the equations for conservation of mass and momentum are thus given by:

$$\nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, \tag{2}$$

$$\nabla \cdot \mathbf{S} = \mathbf{f} \text{ in } \Omega, \tag{3}$$

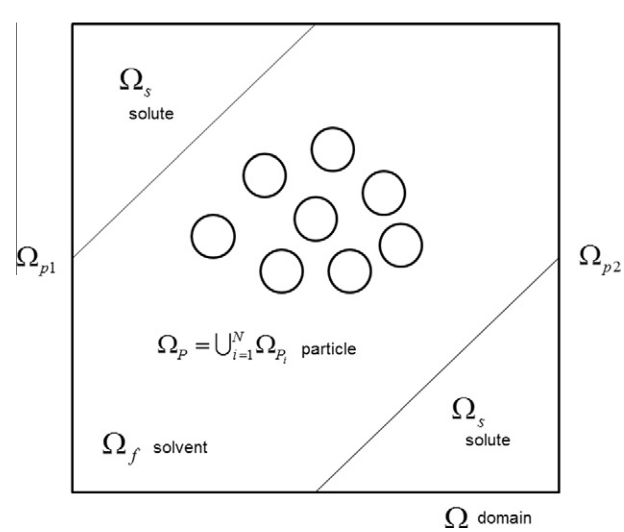

Fig. 1. Schematic diagram for the computation domain of mass transfer in suspending particles.