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Using the direct numerical simulation to compute the slip boundary condition of the solid phase in two-fluid model simulations

Zhi-Gang Feng [a,*], Miguel Enrique Cortina Ponton [a], Efstathios E. Michaelides [b], Shaolin Mao [c]

[a] Department of Mechanical Engineering, University of Texas at San Antonio, San Antonio, TX 78259, United States
[b] Department of Engineering, Texas Christian University, Fort Worth, TX 76129, United States
[c] Department of Mechanical Engineering, University of Texas at Al Paso, El Paso, TX 79968, United States

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ABSTRACT

The simulation of particulate flows for industrial applications often requires the use of two-fluid models, where the solid particles are considered as a separately continuous phase. One of the underlining uncertainties in the use of the two-fluid models in multiphase computations comes from the boundary condition of the solid phase. Typically, the gas or liquid fluid boundary condition at a solid wall is the so called *no-slip* condition, which has been widely accepted to be valid for single-phase fluid dynamics provided that the Knudsen number is low. However, the boundary condition for the solid phase is not well understood. The no-slip condition at a solid boundary is not a valid assumption for the solid phase. Instead, several researchers advocate a slip condition as a more appropriate boundary condition. However, the question on the selection of an exact slip length or a slip velocity coefficient is still unanswered. Experimental or numerical simulation data are needed in order to determinate the slip boundary condition that is applicable to a two-fluid model. In this paper, we investigate the motion of a number of particles near a vertical solid wall, while the particles are in fluidization by a uniform flow. By applying a direct numerical simulation (DNS), the positions and velocities of a total of 500 particles, initially randomly distributed in a 0.20 m × 0.80 m bed, are being tracked and analyzed at each time step. It is found that the motion of particles is highly unsteady. However, the time- and vertical-space averaged values of the particle velocities converge, yielding velocity profiles that can be used to deduce the particle slip length close to a solid wall. The simulation results show a significant amount downward particle slip close to a vertical wall, with the slip velocity increasing as the fluidization velocity increases. However, a negative slip length of approximately 1.2 particle diameters appears to exist. This slip length was found to be insensitive to the values of the fluidization velocity. We also obtained a power–law relationship between the fluidization velocity and fluid/solid fraction, yielding an exponent coefficient of 4.24 for circular particles. The fluidization of 10,000 particles by a jet flow has also been investigated. Significant slip velocity is also observed at the wall.

1. Introduction

Several flow problems in industry and nature involve the flow of a viscous fluid (gas or liquid) with suspended solids. To better understand the dynamics of particulate flows and to aid in the design processes and systems involving particulate flows applications such as fluidized bed reactors, computational simulations provide an efficient, accurate, and inexpensive tool. In the past, researchers have primarily applied two models for studying particulate flows: the classical Eulerian–Eulerian continuum model or two-fluid model [7,17] and the Eulerian–Lagrangian model [5]. The *T*wo-*F*luid *M*odel (TFM) treats the dispersed solid phase as a separate continuum with its own set of governing equations for the momentum equations; both phases have their own physical properties. The traditional Eulerian–Lagrangian model is often called the *D*istinct *E*lement *M*ethod (DEM) or the *UnR*esolved *D*iscrete *P*article *M*ethod (URDPM) [29]; it treats the fluid as a continuum phase and the solid phase as a collection of discrete particles that obey Newton's 2nd law. To determine the velocity and position of a particle, one needs to have the correct value of all the forces acting on the particle, which requires empirical equations for the drag and lift coefficients. Another numerical approach for studying particulate flows is the direct numerical simulation (DNS) method, also termed as the *R*esolved *D*iscrete *P*article *M*ethod (RDPM). This approach resembles the DEM; however, the DNS determines the drag forces on the particles directly by modeling the particles in the flow and solving the fluid governing equations with the proper boundary conditions on the fluid–particle interfaces. Several numerical schemes that can be classified as DNS have been developed in the past decade, including mesh adaption based methods [8,16]; more efficient immersed boundary (IB) based methods [10,23,28] and fictitious domain method [15]. The DNS has been recently extended to include

* Corresponding author. Tel.: +1 210 458 5737; fax: +1 210 458 6504.
E-mail address: zhiang.feng@utsa.edu (Z.-G. Feng).

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particle–fluid heat interactions by obtaining the fluid temperature fields surrounding the particles and computing from the energy equation the heat transfer rate directly [11,12,30]. By taking into account the energy interactions, the DNS method can successfully model the natural convection that occurs around the particles during particulate heat transfer and combustion processes.

As with the solution of all differential equations, the boundary conditions at the wall play a very important role in the accuracy of the results of two-fluid models. Essentially, the boundary conditions define the solution of the particulate flow system. However, there have been very few studies that address quantitatively the problem of the definition of the boundary conditions at the wall for the particulate phase in two-fluid models. Clearly, because of the kinematic non-penetration condition, the normal component of the particulate velocity at the wall must be zero, but there is no *a priori* reason for the tangential velocity component to vanish. Actually, most of the evidence, which includes experimental work and numerical simulations, shows that the tangential no-slip condition is not the right boundary condition for the particulate phase close to solid walls [18,20,21,26]. This phenomenon is also corroborated by the molecular dynamics simulations on the interactions of spheres/molecules with walls in rarefied flows. While the no-slip boundary condition at the walls has been the standard boundary condition for fluid flows, it has been known since the 1920s that there is a slip at the walls in rarefied flows [20]. Brenner and Ganesan [4] provided an insightful view on boundary conditions for any continuum formulation. It is apparent that more information is needed for the behavior of particles near the boundary walls, which will enable us to extract meaningful and accurate boundary conditions for the particulate phase. This information may come from experimental data and DNS studies. The detailed results from the DNS have been proven to be useful in extracting constitutive equations and closure laws that can be employed in DEM or TFM. Pan et al. [22] conducted a DNS of the fluidization of 1204 spherical particles. They were able to successfully simulate the experiment and reproduce the celebrated correlations of Richardson and Zaki (1954), which account for the concentration of particles in the sedimentation process.

The present study pertains to the behavior of solid particles close to a vertical wall from which the normal and tangential velocities of individual particles may be calculated. We have developed a DNS method to simulate a two-dimensional fluidized bed reactor (FBR) and applied this method to groups of particles that circulate in the FBR. From the flow information obtained, we studied the velocities and the overall motion of the particles in the FBR and extracted the time-averaged velocity profile of the particles. The results of the calculations enable us to determine the tangential component of the velocity of the solid phase and its gradient close to the wall and to deduce the slip wall boundary condition that may be used in two-fluid models.

2. The numerical simulation method: DNS

The DNS method that is applied in this study makes use of the IB method takes into account the natural convection around the particles and has been described before by Feng and Michaelides [11]. However, because we wish to study the boundary conditions without the heat transfer complications, in this study we only use the isothermal part of the DNS method. The IB makes use of two geometric domains: the domain of the entire fluid, Ω, and the domain occupied by the solid particles, $\Sigma(S_i)$. In this section we describe briefly the governing equations for the motion of the fluid and of the particles.

The velocity field in the entire domain, Ω, is described by the following equation

$$\frac{\partial \vec{u}}{\partial t}+\vec{u}\cdot\vec{\nabla}\vec{u}=-\vec{\nabla}p+\frac{1}{Re}\nabla^2\vec{u}+\vec{f},\ \vec{x}\in\Omega, \tag{1}$$

where f is the fictitious force exerted by the particles on the fluid domain and the Reynolds number, Re is based on the characteristic velocity and length of the problem,

$$Re=\frac{\rho_f u_{ref} l_{ref}}{\mu_f}. \tag{2}$$

The force density field, in the domain occupied by each particle S_i, can be written by

$$\vec{f}=\frac{\partial \vec{u}}{\partial t}+\vec{u}\cdot\vec{\nabla}\vec{u}+\vec{\nabla}p-\frac{1}{Re}\nabla^2\vec{u},\ \vec{x}\in\sum S_i. \tag{3}$$

The force density is set to zero in the fluid region.

The continuity equation for the entire flow domain Ω is

$$\vec{\nabla}\cdot\vec{u}=0,\ \vec{x}\in\Omega \tag{4}$$

The velocity field inside the region occupied by the solid particles, $\Sigma(S_i)$ can be computed by

$$\vec{u}=\vec{U}_p+\vec{\omega}_p\times\left(\vec{x}-\vec{x}_p\right), \tag{5}$$

where $\vec{x}_p$ is the position vector of the center of mass of the particle. Eq. (5) ensures that the particles undergo a solid body motion. Based on the results for the entire flow domain, the linear and angular velocities of each particle in the flow field are computed at every step of the simulation according to the following expressions:The particle velocity is obtained from the force balance around the fluid at the interface with the particle. The force balance results in the following expression:

$$\rho_p V_p\frac{d\vec{U}_p}{dt}=\rho_f\oint_{\partial s}\tilde{\sigma}\cdot d\vec{s}+\int_s\left(\rho_p-\rho_f\right)\vec{g}\,dv, \tag{6}$$

where $\rho_p,\rho_f,V_p,\vec{U}_p,\tilde{\sigma}$ are particle and fluid density, particle volume, linear velocity and fluid stress tensor respectively.

The surface integral of Eq. (6) may be evaluated with the application of the Cauchy theorem and becomes:

$$\rho_f\oint_{\partial s}\tilde{\sigma}\bullet d\vec{s}=\rho_f\int_s\vec{f}\,dv+\rho_f\frac{d}{dt}\int_s\vec{u}\,dv. \tag{7}$$

The time derivative of the volume integral in the last expression may be simplified as follows:

$$\frac{d}{dt}\int_s\rho_f\vec{u}\,dv=\rho_f V_p\frac{d\vec{U}_p}{dt}. \tag{8}$$

Substituting Eqs. (7) and (8) into Eq. (6) the following expression for the linear motion of the particle may be derived:

$$\left(\rho_p-\rho_f\right)V_p\frac{d\vec{U}_p}{dt}=\rho_f\int_s\vec{f}\,dv+\left(\rho_p-\rho_f\right)V_p g\vec{e}_y, \tag{9}$$

where g is the gravitational acceleration constant and $\vec{e}_y$ is the unit vector in the direction of the gravity force.

The angular velocity of the particles is given by the balance of the moments around the particles as follows:

$$\frac{1}{2}\pi r^4\rho_p\frac{d\vec{\omega}_p}{dt}=\rho_f\oint_{\partial s}\left(\vec{x}-\vec{x}_p\right)\times\left(\tilde{\sigma}\cdot d\vec{s}\right), \tag{10}$$

where $\vec{\omega}_p$ and r are the angular velocity and the radius of the particle respectively.