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Lattice Boltzmann based discrete simulation for gas–solid fluidization

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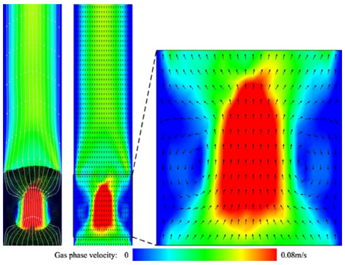
HIGHLIGHTS

- Lattice Boltzmann based discrete particle simulation is proposed and validated.
- The EMMS drag has been coupled with lattice Boltzmann based DPS.
- The modified LBE restores the effect of porosity and slip velocity on gas flows.
- LES incorporated into the LBM to model turbulence in gas–solid fluidization.
- The proposed method is able to simulate the size of particles below millimeter.

GRAPHICAL ABSTRACT

The governing equations of gas flow in DPS are described by a modified LBE with a reasonable consideration of the effect of both the local solid volume fraction and the local relative velocity between particles and fluid rather than the volume-averaged Navier–Stokes equations. A gas phase leaves the roof of bubble, and the downward moving particles near wall drag the gas to the bottom of the bubble where it re-enters the bubble region, which results in a pair of symmetrical vortices can be observed in the neighborhood of the rising bubble (Snapshots of the detailed flow field for gas phase).



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ABSTRACT

Discrete particle simulation, a combined approach of computational fluid dynamics and discrete methods such as DEM (discrete element method), DSMC (direct simulation Monte Carlo), SPH (smoothed particle hydrodynamics), PIC (particle-in-cell), etc., is becoming a practical tool for exploring lab-scale gas–solid systems owing to the fast development of parallel computation. However, gas–solid coupling and the corresponding fluid flow solver remain immature. In this work, we propose a modified lattice Boltzmann approach to consider the effect of both the local solid volume fraction and the local relative velocity between particles and fluid, which is different from the traditional volume-averaged Navier–Stokes equations. A time-driven hard sphere algorithm is combined to simulate the motion of individual particles, in which particles interact with each other via hard-sphere collisions, the collision detection and motion of particles are performed at constant time intervals. The EMMS (energy minimization multi-scale) drag is coupled with the lattice Boltzmann based discrete particle simulation to improve the accuracy. Two typical fluidization processes, namely, a single bubble injection at incipient fluidization and particle clustering in a fast fluidized bed riser, are simulated with this approach, with the results showing a good agreement with published correlations and experimental data. The capability of the approach to capture more detailed and intrinsic characteristics of particle–fluid systems is demonstrated. The method can also be used straightforward with other solid phase solvers.

1. Introduction

Gas–solid fluidization systems are widely encountered in both physical and chemical processes for many industries, for instance,

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fluid catalytic cracking (FCC), circulating fluidized bed combustion (CFBC), coal gasification, and sulfide roasting. Earlier studies of these systems mainly focused on experimental investigations including measurement of macroscopic hydrodynamic behavior and development of some corresponding correlations. In recent decades, to quantitatively understand the complex hydrodynamics of gas–solid fluidization, the computational fluid dynamics approach is adopted in many cases, and a lot of numerical methods in the hydrodynamic modeling and simulation of gas–solid fluidization at different levels have been proposed, such as two-fluid model (TFM) (Anderson and Jackson, 1967; Ishii, 1975), quadrature-based moment methods (QBMM) (Fox, 2008, 2009a, b; Desjardins et al., 2008), discrete particle simulation (DPS) (Tsuji et al., 1993; Hoomans et al., 1996; Xu and Yu, 1997), and direct numerical simulation (DNS) (Hu et al., 1992; Ma et al., 2006; Wang et al., 2010; Xiong et al., 2012).

Among these numerical methods, the most frequently used TFM treats the gas and solid phases as two interpenetrating continua, and locally averaged quantities such as volume fractions, velocities, species concentrations, and temperatures of gas and solid phases appear as dependent field variables (Anderson and Jackson, 1967; Ishii, 1975). To derive TFM using ensemble averaging techniques, terms such as effective stresses and inter-phase interaction have to be introduced, which require constitutive equations for closure. Only under very limited conditions, those constitutive equations can be obtained rigorously from the kinetic theory of granular flow (Gidaspow, 1994), otherwise we have to resort to empirical models. The accuracy and effectiveness of TFM are, therefore, still unsatisfactory in many circumstances. The recently developed QBMM permits to solve population balance equation (PBE) in commercial CFD codes at relatively low computational cost. However, its application to the context of multiphase flows is to be explored (Mazzei, 2011). Comparably, DNS not only fully resolves the motion of each individual solid particle and fluid flow, but also directly calculates the hydrodynamic force acting on each individual solid particle from the stress on the fluid–solid boundary. Due to its capability in detailed solution around each particle, DNS has been regarded as the most accurate method for the simulation of gas–solid flows. Unfortunately, DNS is too costly for predicting the hydrodynamics in large industrial scale fluidized beds even at low Reynolds numbers, let alone the high Reynolds number cases where their grid size and time step are limited by the Kolmogorov length scale and the turbulence time scale (Xiong et al., 2012).

For numerical modeling of gas–solid fluidized beds mentioned above, TFM is computationally more economic but inaccurate, while DNS is computationally more accurate but expensive. So it is natural to ask whether there exists a better alternative combining the advantages of the two methods for modeling the gas–solid flows. As a particle-scale approach, DPS is somehow in between these two ends and seems to give a good balance among accuracy, cost and efficiency. Specifically, DPS resolves the continuum fluid flow at the scale of computational cells in CFD, describes the motion of individual particles by the well-established Newton's equations of motion, and models particle–particle interactions through different collision models such as the hard-sphere model and the soft-sphere model, which has been proven to be effective in modeling various particle flow systems (Deen et al., 2007; Zhu et al., 2007, 2008), such as slugging fluidized bed (Xu et al., 2007), spouted bed (Zhao et al., 2008), pneumatic conveying (Kuang et al., 2008), bubbling fluidized bed (Geng and Che, 2011), sound-assisted fluidized bed (Wang et al., 2011), and cyclone separator (Chu et al., 2011). However, in all these mentioned work, the fluid motion with suspended solids is commonly governed by the volume-averaged Navier–Stokes equations or their simplified forms (Tsuji et al., 1993; Hoomans et al., 1996; Xu and Yu, 1997; Mikami et al., 1998), and those equations are solved based on implicit schemes no matter by Fluent (Chu and Yu, 2008a,b; Chu et al., 2009a,b, 2011; Wu et al., 2010; Zhao et al., 2010), OpenFOAM (Su et al., 2011; Goniva et al., 2012), MFIX (Darabi et al., 2011; Garg et al., 2012; Li and Guenther, 2012; Li et al., 2012a,b; Gopalakrishnan and Tafti, 2013), or in-house codes (Ouyang and Li, 1999a,b, Zhou et al., 2004a,b; Zhao et al., 2009; Wang et al., 2009; Wu et al., 2009). With implicit methods the discretized equations are solved simultaneously, which inevitably requires some kind of global data dependence and hence global communication. Therefore, most algorithms involved suffer from relatively lower scalability and parallel efficiency, which becomes a grand challenge for fast simulation of large-scale industrial systems.

As a smoothed alternative to lattice gas automata (LGA), lattice Boltzmann method (LBM) (McNamara and Zanetti, 1988) is an efficient second-order flow solver capable of solving various systems for hydrodynamics owing to its explicit solution of particle distribution function, algorithmic simplicity, natural parallelism, and flexibility in boundary treatment (Chen and Doolen, 2003). Therefore, LBM becomes an increasingly popular approach to simulation of complex flows (Aidun and Clausen, 2010) and can be easily incorporated into DPS. Filippova and Hanel (1997) proposed a combination of lattice-BGK model and Lagrangian approach, and performed three-dimensional simulation of gas–particle flow through filters with one-way coupling, where the fluid affected the particles but the particles did not affect the fluid. Chen et al. (2004) simulated particle-laden flow over a backward-facing step with two-way coupling, where a modified lattice-BGK model was developed for the fluid flow and a Lagrangian approach for particles. But they did not consider the effect of solid volume fraction on gas flows. Sungkorn et al. (2011) proposed a gas–liquid Lagrangian-LBM to simulate turbulent gas–liquid bubbly flows with a relatively low gas holdup. Specifically, they solved the continuous liquid phase by single-phase lattice Boltzmann equation (LBE) incorporated with large eddy simulation (LES) (Smagorinsky, 1963), and evolved the dispersed gas phase (i.e. the individual bubbles) by Lagrangian trajectories, but did not include the gas volume fraction in the conservation equations and its effect on drag force.

In this paper, we proposed a modified LBE to model the fluid flow and developed the corresponding fluid–solid interaction model in the framework of DPS. The effects of both the local solid volume fraction and local relative (slip) velocity between particles and fluid are considered. The equations of motion governing individual particles are solved with time-driven hard-sphere (TDHS) model. It is noteworthy that the computational strategy herein has ever been implemented in direct simulation of particle–fluid systems (Wang et al., 2010) where the modified LBE was used with particle size much larger than the cell spacing. In the present work, the partial saturation concept has been extended to model the objects much smaller than the cell spacing (i.e. porous media), and both the linear and nonlinear drag effects of the solid phase (media) have been considered in the lattice Boltzmann based discrete particle simulation for the first time.

2. Numerical approach

The objective of this research is to develop a lattice Boltzmann based numerical method for discrete simulation of gas–solid fluidization systems. For illustration, we used two-dimensional nine-velocity (D2Q9) lattice Boltzmann model as an example, and the solid particles distributed in the lattice cell were described by the time-driven hard sphere model. A schematic diagram of this method is shown in Fig. 1.