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Simulation of flow behavior of liquid and particles in a liquid–solid fluidized bed

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ABSTRACT

Flow behavior of liquid and solid phases is simulated by means of DEM-CFD in a liquid–solid fluidized bed. The lubrication force is considered. A detailed description of the model equations used has been presented. The distributions of velocity and volume fraction are predicted at the different superficial liquid velocities, liquid viscosity and solids densities in the bed. The granular temperature is computed from simulated particle velocity. Predicted solid axial velocities are in agreement with experiments. Simulations indicate that axial velocities of particles increase with the increase in the superficial liquid velocity. The bed expansion height is increased with an increase of superficial liquid velocity and liquid viscosity and decreases with the increase of particle density. The lubrication force reduces granular temperature in the liquid–solid fluidized beds.

1. Introduction

Solid–liquid fluidized beds have been widely used in industry for hydrometallurgical operations, catalytic cracking, ion exchange, adsorption, crystallization, sedimentation, particle classification, etc. [1,2]. In the design of these solid–liquid fluidized beds, it is important to understand and have an ability to predict the bed expansion and particle mixing. These characteristics govern the equipment volume depending upon the phase in which the reaction (and/or the mass transfer) takes place. Further, the spatial distribution of solid phase hold-up governs the flow pattern of solid and liquid phases and thus indirectly affects the extent of intermixing and the rates of mass and heat transfer.

As regards to mathematical modeling, computational fluid dynamic (CFD) simulations of the flow in fluidized beds gives very detailed information about the local values of phase hold-ups and their spatial distributions, liquid phase flow patterns and the intermixing levels of the individual phases especially in the regions where measurements are either difficult or impossible to obtain. Such information can be useful in the understanding of the transport phenomena in fluidized beds. In numerical simulation of fluidized beds, Eulerian–Lagrangian models describe the fluid flow using the continuum equations, and the particulate phase flow is described by tracking the motion of individual particles [3–5]. Discrete particle models (DPM) have been used for a wide range of applications involving particles ever since it was first proposed by Cundall and Strack [6]. A major difference with these traditional DPM models is that a detailed description of the gas-phase dynamics is required, in order to describe the interaction between the particles and the fluid phase. The coupling of the DPM with a finite volume description of the gas-phase based on the Navier–Stokes equations was first reported in the open literature by Tsuji et al. [7] and Hoomans et al. [8] for the soft-sphere model and the hard sphere model respectively. In a hard-sphere system the trajectories of the particles are determined by momentum-conserving binary collisions. The interactions between particles are assumed to be pair-wise additive and instantaneous. In the simulation, the collisions are processed one by one according to the order in which the events occur. Note that the possible occurrence of multiple collisions at the same instant cannot be accounted for. At high particle number densities, the collisions will lead to a dramatical decrease in kinetic energy. This is the so-called inelastic collapse McNamara and Young [9], in which regime the collision frequencies diverge as relative velocities vanish. Clearly in that case, the hard-sphere method becomes useless.

In more complex situations, the particles may interact via short- or long-range forces, and the trajectories are determined by integrating the Newtonian equations of motion. The soft-sphere models use a fixed time step and consequently the particles are allowed to overlap slightly. The contact forces are subsequently calculated from the deformation history of the contact using a contact force scheme. The soft-sphere models or discrete element method (DEM) allow for multiple particle overlap although the net contact force is obtained from the addition of all pair-wise interactions. The soft-sphere models are essentially time driven, where the time step should be carefully chosen in the calculation of the contact forces. DEM-CFD simulations of single solid species in liquid-particle flows were carried by Apostolou and Hrymak [10], showing the ability to capture representative behaviors of the two-phase flow. For binary mixtures fluidized by a liquid, a statistical mechanics model, developed by Seibert and Burns [11], was shown to be able to capture

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the expansion behavior as well as some features of the components' distribution along bed height. Mukherjee and Mishra [12], by a simplified hydrodynamics combined to DEM, proved the capability of their model to reproduce qualitatively the layer inversion phenomenon for selected binaries fluidized by water. Agreement, again only in qualitative terms, of DEM-CFD simulations with physical observations of layer inversion in liquid-fluidized beds has also been reported by Zhou and Yu [13], who adapted a mono-disperse drag law to account for the presence of a two-size mixture. Renzo et al. [14] predicted the layer inversion by means of DEM-CFD in a liquid–solid fluidized bed. The simulations not only demonstrate the importance of correctly accounting for the local size distribution in the bed, but also prove the validity of the overall computational approach. The predictions of the simulations depend on the system considered, both in terms of critical velocity and, expansion of the individual components in the bed. Definitely, DEM-CFD may allow to investigate the local particle flow field, highlighting the motion of particles in apparently chaotic vortices continuously forming and disappearing, which is thought to be the mechanism responsible for mixing of particles in the bed. However, detailed and quantitative comparisons with published experimental data are still lacking.

With regards to mathematical modeling, CFD simulations of the flow in liquid–solid fluidized beds gives very detailed information about the local values of concentrations and their spatial distributions, especially in the regions where measurements are either difficult or impossible to obtain. Such information can be useful in the understanding of the transport phenomena in liquid–solid fluidized beds. Though a large number of numerical simulations and experimental observations have been made, to understand the hydrodynamics in liquid–solid fluidized beds is still required. Quantitative understanding is also needed to explain the effects of liquid velocity and particles sizes. In this study, DEM is used to simulate the liquid–solid two-phase flow. The hydrodynamics of liquid–solid fluidized bed is analyzed to understand the flow phenomena.

2. Eulerian–Lagrangian gas–solid flow model

The DEM-CFD approach is relatively well documented in the literature [3–5,13], so here the salient features of the model equations used will be summarized. Our DEM-CFD implementation uses a rather standard coupled approach based on the particle-scale Discrete Element Method for the solid phase [6] and a local average CFD approach for the fluid phase [8].

2.1. Equation of motion for liquid phase

Generally in numerical simulation of fluid flow, the fluid motion is considered two-dimensionally as a function of *t*, *x* and y. The fluid phase flow is solved by a locally averaged approximation of the continuity and Navier–Stokes equations with an averaging scale of the order of the computational cell (typically a few particle diameters). The equations of conservation of mass and momentum are:

$$\frac{\partial(\rho_l\varepsilon_l)}{\partial t}+\nabla\cdot(\rho_l\varepsilon_l\boldsymbol{u}_l)=0 \tag{1}$$

$$\frac{\partial(\rho_l\varepsilon_l\boldsymbol{u}_l)}{\partial t}+\nabla\cdot(\rho_l\varepsilon_l\boldsymbol{u}_l\boldsymbol{u}_l)=-\varepsilon_l\nabla P+\varepsilon_l\nabla\cdot\tau_l+\varepsilon_l\rho_l\mathbf{g}-F_{pl} \tag{2}$$

where g is the acceleration due to gravity, P the liquid pressure, ε_l the liquid volume fraction, and τ_l the viscous stress tensor. The coupling term F_{pl} between the particle phase and liquid phase is estimated as the sum of the drag on each particle within the corresponding fluid control volume. The stress tensor of liquid phase can be represented as

$$\tau_l=\mu_l\left[\nabla\boldsymbol{u}_l+(\nabla\boldsymbol{u}_l)^T\right]-\frac{2}{3}\mu_l(\nabla\cdot\boldsymbol{u}_l)\boldsymbol{I} \tag{3}$$

where μ_l is the viscosity of liquid phase.

2.2. Equation of motion for a particle

Spherical particles of uniform size are investigated in present work. The particles are tracked individually by the Newton's second law of motion. Each particle has two types of motion, translational and rotational motions. The motion of each individual particle is governed by the laws of conservation of linear momentum (Newton's second law of motion) and angular momentum, expressed, for the *i*-particle, by

$$m_i\frac{d\boldsymbol{v}_i}{dt}=-V_p\nabla P+m_i\boldsymbol{g}+f_d+f_m+f_l+f_c \tag{4}$$

$$I_p\frac{d\boldsymbol{\omega}}{dt}=T_p \tag{5}$$

where m_i and v_i are the mass and velocity of a particle, V_p is the volume of a particle in the liquid cell, ρ_i is the density of liquid . The terms of the right-hand side of Eq. (4) are the liquid pressure gradients, gravity, drag force exerted from the fluid, virtual mass force, lubrication force and contact force. T_p is the torque arising from the tangential components of the contact force. I_p and ω are the moment of inertia and angular velocity of a particle.

The liquid–solid interaction force, or drag force, is determined at each particle. The drag force depends on not only the relative velocity between the solid particle and fluid but also the presence of neighboring particles, i.e., local volume fraction of solid phase. The drag force is expressed by considering these factors as follows:

$$f_d=\frac{\beta V_p}{1-\varepsilon_l}\left(u_l-u_p\right) \tag{6}$$

where ε_l and β are the volume fraction of fluid and an inter-phase momentum transfer coefficient. A proper drag model for the description of β is vital in solid–fluid interaction problems. The correlations given by Gidaspow [15] are often used. The correlation is a combination of the works of Ergun [16] and Wen and Yu [17]; the formulation presented by Ergun [16] is used at the liquid volume fraction less than 0.8 where the suspension is dense, whereas the formulation by Wen and Yu [17] is used at the liquid volume fraction greater than 0.8 where the suspension is dilute.

$$\beta_E=150\frac{(1-\varepsilon_l)^2\mu_l}{(\varepsilon_l d_s)^2}+1.75\frac{\rho_l(1-\varepsilon_l)|\mathbf{u}_l-\mathbf{u}_s|}{\varepsilon_l d_s}\qquad \varepsilon_l\le 0.8 \tag{7a}$$

$$\beta_{WY}=\frac{3}{4}C_d\frac{\rho_l(1-\varepsilon_l)|\mathbf{u}_l-\mathbf{u}_s|}{d_s}\varepsilon_l^{-2.65}\qquad \varepsilon_l>0.8 \tag{7b}$$

$$C_d=\begin{cases}\dfrac{24}{\mathrm{Re}}\left(1+0.15\mathrm{Re}^{0.687}\right) & \mathrm{Re}\le 1000\\ 0.44 & \mathrm{Re}\ge 1000\end{cases} \tag{8}$$

The transition proposed by Gidaspow [15] makes the drag law discontinuous in liquid volume fraction it is continuous in Reynolds number. Physically, the drag force is a continuous function of both solid volume fraction and Reynolds number, and therefore the continuous forms of the drag law may be needed to correctly simulate liquid–solid fluidized beds. To avoid discontinuity of these two correlations, a switch function φ is introduced to give a smooth from the dilute regime to the dense regime [18]

$$\varphi=\frac{\arctan\left[150\times 1.75\left(0.2-\varepsilon_p\right)\right]}{\pi}+0.5 \tag{9}$$

Thus, the interface momentum transfer coefficient becomes

$$\beta=(1-\varphi)\beta_E+\varphi\beta_{WY} \tag{10}$$