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Numerical simulation of gas–solid fluidized beds by coupling a fluid-dynamics model with the discrete element method

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ABSTRACT

Gas–solid fluidization is not only an essential phenomenon in many areas of industry, but is also used to understand particle behavior in a number of research fields. For the safety analysis of core disruptive accidents in liquid-metal fast reactors, a hybrid method is developed by combining the discrete element method with a fluid-dynamics model of the reactor safety analysis code SIMMER-III to reasonably simulate particle transient behavior, as well as the occurring thermal-hydraulic phenomena. As a preliminary validation procedure, the developed hybrid method is applied to simulations of gas–solid two-phase flows. In this study, numerical simulations of two typical gas–solid fluidized bed systems are performed. The particles in the beds are porous alumina of 70 μm diameter and glass of 530 μm diameter, which belong to Geldart groups A and B, respectively. The reasonable agreement between our simulation results and experimental data from the literature demonstrates the fundamental validity of the present simulation method for multiphase flows with large amounts of solid particles.

1. Introduction

Gas–solid fluidized beds are complicated multiphase problems. They are not only considered to be essential phenomena in many industry areas, such as catalytic reactions and ore calcination, but are also used to understand particle behavior and gas-phase characteristics in a number of research fields.

To simulate gas–solid fluidization behavior reasonably, it is necessary to consider the interaction between the gas phase and particles, as well as the interaction between particles themselves, in an appropriate manner. Even now, it is difficult to exactly simulate strong interactions between particles and between particles and the solid walls of a system in multiphase flows. In macro-scale computational methods, which are usually built on an Eulerian framework, particles in a fluidized bed can be treated as a kind of fluid. Therefore, in the majority of related literature, the continuum assumption is applied to the particle phase. For example, the two-fluid model (TFM) (Jackson, 1963) regards the particle–fluid mixture as the blending of two fluids, and this can predict the time-averaged and instantaneous porosities of the mixture well (Yuu et al., 2000). To date, TFM has successfully described the hydrodynamics of two characteristic groups of particles, namely Geldart groups B and D (Mazzei and Lettieri, 2008). However, the constitutive relations used in this model are usually based on empirical equations, and hence lack generality under the limits of model application. Under the Eulerian framework, the computational domain is composed of multiple mesh cells, and physical variables in each cell are assumed to be uniform for the particle phase. When a cell has a high volume fraction in the particle phase, it is always difficult to represent the strong interaction between particles, as well as the discrete particle characteristics, using the continuum model. The other category of numerical methods treats particles discretely at a mesoscopic level. Among them, the development of the discrete element method (DEM), introduced by Cundall and Strack (1979), is the most active field. With an explicit force model, multi-body collisions can be calculated directly and exactly. In addition, DEM provides local transient information about particles, such as their trajectories and velocities. Various numerical studies have applied DEM to the numerical simulation of fluidized beds (Tsuji et al., 1993; Yuu et al., 2000).

The consideration of gas–particle interactions is another difficulty in numerical simulations. In Eulerian–Eulerian approaches such as TFM, the solution depends significantly on a proper

Abbreviations: TFM, the two-fluid model; DEM, discrete element method; CFD, computational fluid dynamics; CDAs, core disruptive accidents; LMFRs, liquid-metal fast reactors.

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description of the interfacial force and solid stress acting on particles (Pei et al., 2012). On the other hand, it is more straightforward to couple the DEM with a computational fluid dynamics (CFD) method in a multi-scale modeling scheme, based on an Eulerian–Lagrangian framework. In this coupling method, the gas phase is modeled as a continuum, and is solved based on the Eulerian description. With this in mind, Tsuji et al. (1993) introduced a DEM–CFD coupling algorithm, and then the CFD–DEM methods have been widely used in the simulation of multiphase flows.

When core disruptive accidents (CDAs) occur in liquid-metal fast reactors (LMFRs), core debris may settle on the core-support structure and form conic bed mounds. Heat convection and vaporization of coolant sodium will then level this debris bed. To reasonably simulate such transient behavior, as well as thermal-hydraulic phenomena occurring during a CDA, a comprehensive computational tool is needed. SIMMER-III (Yamano et al., 2003) is a successful computer code that was developed as an advanced tool for CDA analysis in LMFRs. It is a 2D, multi-velocity-field, multiphase, multicomponent, Eulerian fluid dynamics code coupled with a fuel-pin model and a space- and energy-dependent neutron kinetics model. In recent decades, the SIMMER code has been successfully applied to simulations of key thermal-hydraulic phenomena involved in CDAs, as well as to assessments of reactor safety. However, in simulations of multiphase flows with large amounts of solid particles, the fluid-dynamics models of SIMMER-III do not consider strong interactions among solid particles or the particle characteristics. Therefore, a hybrid computational method is developed by combining DEM with the fluid-dynamics model of SIMMER-III. This approach reasonably simulates the particle behavior, as well as the thermal-hydraulic phenomena, in CDAs. In the coupling algorithm, the governing equations of the gas phase are solved by a semi-implicit time-factorization approach, whereas particle movements are calculated using DEM. The two phases are then explicitly coupled through drag force terms in their governing equations.

As a preliminary validation procedure, the developed hybrid method is applied to simulations of gas–solid two-phase flows. In this study, numerical simulations of two typical gas–solid fluidization systems consisting of Geldart group A and B particles (Geldart, 1973) are performed, and the numerical results are compared with experimental data from the literature.

2. Mathematical treatment

2.1. Governing equations

If the heat transfer between two phases can be neglected, the governing equations of the gas phase are the conservation equations of mass and momentum in terms of the local mean variables over a computational cell. These can be expressed in the following abbreviated form:

$$\frac{\partial \alpha_g \rho_g}{\partial t} + \nabla \cdot \left(\alpha_g \rho_g \cdot \vec{v}_g \right) = 0 \tag{1}$$

$$\frac{\partial \alpha_g \rho_g \vec{v}_g}{\partial t} + \nabla \cdot \left(\alpha_g \rho_g \vec{v}_g \vec{v}_g \right) = -\alpha_g \nabla p + \alpha_g \rho_g \vec{g} + \vec{S}_d + \nabla \cdot \left(\alpha_g \hat{\tau}_g \right) \tag{2}$$

where the subscript g denotes the gas phase, t is time, α_g, ρ_g, and $\vec{v}_g$ are the void fraction, gas density, and velocity, respectively, $\hat{\tau}_g$ is the viscous stress tensor expressed by Newton's law of viscosity, $\vec{g}$ is the gravitational acceleration, and $\vec{S}_d$ is the momentum exchange term between particle and gas phases.

The particle phase is treated as discrete, and the motion of particle i is described by Newton's law of motion as follows:

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_{c,i} + \vec{F}_{f,i} + \vec{F}_{g,i} \tag{3}$$

$$\vec{v}_i = \frac{d\vec{r}_i}{dt} \tag{4}$$

$$I_i \frac{d^2 \vec{\theta}_i}{dt^2} = \sum_j \vec{A}_{ij} \tag{5}$$

$$\vec{\omega}_i = \frac{d\vec{\theta}_i}{dt} \tag{6}$$

where m_i, $\vec{r}_i$, $\vec{v}_i$, I_i, $\vec{\theta}_i$, and $\vec{\omega}_i$ are the mass, position, translation velocity, moment of inertia, angular displacement, and velocity of particle i, respectively, $\vec{F}_{c,i}$ is the contact force between particle i and its neighbor particle or wall, $\vec{F}_{f,i}$ denotes the total particle–gas interaction force for particle i, $\vec{F}_{g,i}$ is the gravitational force of particle i, and $\vec{A}_{ij}$ is the torque between particles i and j.

2.2. Fluid dynamics algorithm

The overall fluid-dynamics solution of the SIMMER-III code for gas and particle phases is based on a time-factorization time-splitting approach. This is the four-step algorithm developed for the advanced fluid-dynamics model (Bohl et al., 1990). In Step 1 of this algorithm, intra-cell transfers are solved without considering the convection terms. In Step 2, the end-of-time-step variables are explicitly estimated to initialize the pressure iteration. In Step 3, the pressure iteration is conducted to obtain consistent velocity and pressure using a multivariate Newton–Raphson method. The iterative calculations in this step are strictly controlled to reduce the residuals of selected sensitive variables to zero. Finally, in Step 4, consistent mass and momentum convections are computed based on a semi-implicit method.

2.3. Methodology of DEM

Under the assumption of DEM, particles in 2D systems are assumed to be circular. The contact forces between the particles, as well as between particles and the wall, are calculated by applying a viscoelastic contact model (Balevičius et al., 2008). For a particle i, the contact force $\vec{F}_{c,i}$ is divided into the normal and tangential components.

$$\vec{F}_{c,i} = \sum_j \vec{F}_{c,ij} = \sum_j \vec{F}_{c,ij,nor} + \sum_j \vec{F}_{c,ij,tan} \tag{7}$$

where the subscript j denotes the neighbor particles of particle i.

The normal component of the contact force $\vec{F}_{c,ij,nor}$ between particles i and j is described by Hooke's contact law as follows:

$$\vec{F}_{c,ij,nor} = \frac{4}{3} \cdot \frac{E_i E_j}{E_i(1-\nu_i^2) + E_j(1-\nu_j^2)} R_{ij} h_{ij} \vec{n}_{ij} - \gamma_{nor} m_{ij} \vec{u}_{ij,nor} \tag{8}$$

where $m_{ij} = \frac{m_i m_j}{m_i + m_j}$ and $R_{ij} = \frac{R_i R_j}{R_j + R_j}$ present the reduced mass and radius, respectively, of particles i and j, E is the Young's modulus, ν is Poisson's ratio, $h_{ij} = R_i + R_j - |\vec{r}_{ij}|$ is the overlap length, $\vec{r}_{ij}$ is the vector of a relative position, $\vec{n}_{ij}$ is the unit vector normal to the contact surface with particle j directed towards particle i, $\vec{u}_{ij,nor}$ is the normal component of the relative contact velocity between particles i and j, and γ_{nor} is the viscous damping coefficient in the normal direction.

The tangential force $\vec{F}_{c,ij,tan}$ is qualified by separating the static and dynamic friction forces as:

$$\vec{F}_{c,ij,tan} = \vec{t}_{ij} \min\left(\left| \vec{F}_{c,ij,\text{static}} \right|, \left| \vec{F}_{c,ij,\text{dynamic}} \right| \right) \tag{9}$$

where $\vec{t}_{ij}$ is the unit tangential vector.