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A coupled Eulerian fluid phase-Eulerian solids phase-Lagrangian discrete particles hybrid model applied to gas-solids bubbling fluidized beds

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ABSTRACT

Because the traditional Eulerian-Eulerian approach and Lagrangian-Eulerian approach are essentially the description of dense gas-solid two-phase flow in two reference frames, it is natural to expect that these approaches are related. A coupled Eulerian fluid phase-Eulerian solids phase-Lagrangian discrete particle phase (CEEL) hybrid approach is proposed where transport equations of fluid phase and Eulerian solids phase are solved in an Eulerian framework and the discrete particle phase is represented as Lagrangian framework. In this CEEL model, the solid phase is described by Eulerian solids phase and Lagrangian discrete particle phase. The ghost phase is introduced to represent either Eulerian solids phase or discrete particle phase as the solid phase. The Eulerian solids phase properties are modeled by means of kinetic theory of granular flow with an impact velocity-dependent restitution coefficient as functions of granular temperature. The collisions of discrete particles are handled using a discrete element method. Simulations are carried out in a dense gas-solid bubbling fluidized bed. The predicted solids flux agrees with the experimental data. Such approaches to closure model building enforce the macroscopic conservation principles while attempting to accommodate local variations in momentum exchange due to bubble formation mechanisms in gas-solid fluidized beds.

1. Introduction

Gas-solid bubbling fluidized beds are widely used in industry for variety of processes, for example coal combustion and gasification, incineration of solid waste and heterogeneously catalyzed reactions, etc. Modeling of the bubbling fluidized beds is challenging due to complexity of the hydrodynamic behavior of gas and solids phases (e.g., [1–11]). Two common approaches, including Eulerian–Eulerian (EE) and Eulerian–Lagrange (EL) methods, are shown in Fig. 1 for modeling gas-solid bubbling fluidized beds.

In the Eulerian–Eulerian approach, referred as the two fluid model (TFM), both the fluid phase and solid phase are treated as interpenetrating continua which leads to a system of averaged Navier–Stokes equations. Early the simulations of solids phase relied on empirical solid viscosity eq. [12,13] and elasticity-type correlation to account for the solid phase normal stresses [14,15]. On the other hand, the Eulerian two-fluid model with kinetic theory of granular flow closure provides a unique approach for the simulation and design of gas–particles fluidized beds. The development of the kinetic theory of granular flow derived from the general theory of non-uniform dense gases [16]. In this approach, the solids phase is formed by uniform spheres and only binary instantaneous collisions are considered (e.g., [17–19]). The basic concept of the theory is the granular temperature. During random oscillations of the particles, the inelastic collisions occur causing energy to be dissipated. The granular temperature measures these random oscillations of particles and is defined as the average of the three variances of the particle's velocities. The effects of the particles interactions on the rheology are modeled by means of the granular temperature. Generally, these kinds of models are more complex and time-consuming to solve, but they are applicable for a wider range of gas-solid fluidized beds. This approach has the advantage of having a deeper phenomenological basis than the early theories, and was reviewed by Gidaspow [20]. The kinetic theory of granular flow is fairly free from empirical constants. The only empirical input that appears directly in the model is the restitution coefficient of particles. The restitution coefficient represents the loss of energy during collision and varies between zero and one. If it is equal to one, there is no energy loss during collision (elastic collision); otherwise, energy is dissipated during collision (inelastic collision). The coefficient of restitution depends, at least, on the material of the particles and on the relative velocity between two colliding particles. As far as the restitution coefficient is concerned, its value affects the results significantly in numerical simulations of gas-solid bubbling fluidized beds.

Eulerian–Lagrange (EL) strategies provide an alternative framework for numerical simulations of gas-solid fluidized beds. In EL approach, the

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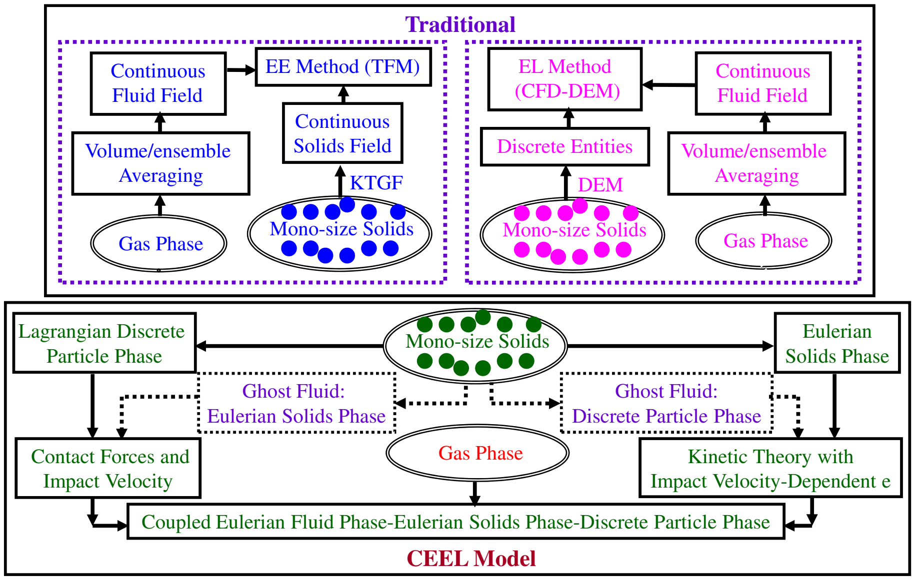

Fig. 1. Different numerical descriptions of modeling of gas-particle fluidized beds.

fluid phase is evolved in the Eulerian framework and the solid phase is treated by the Lagrangian framework. In the Eulerian approach, conservation equations are solved for the fluid mass and momentum per unit volume on a fixed grid. In the Lagrangian framework, equations are solved for the position and momentum of discrete particles that move through the fixed Eulerian grid. These trajectories are used to calculate the collisional forces. These collisions can be stochastically modeled or deterministically detected. In the stochastic-direct simulation Monte Carlo (DSMC) model, the real particles are represented by a lower number of representative particles. The trajectories of only these representative particles are calculated, and the collisions between pairs of particles are detected stochastically [21,22]. Shuyan et al. [23] found that the stochastic collision models by means of DSMC method produce unrealistic results such as solid volume fractions greater than unity in the control volume in a gas-solid riser. For the discrete particle simulations with deterministic collision detection, two models are widely applied: the hard-sphere model and the soft-sphere model. In the hard-sphere model, single binary collisions are considered as instantaneous processes (e.g., [24,25]). In the soft-sphere model, also known as discrete element method (DEM), the particles can overlap each other or penetrate into the wall (e.g., [26–32]). The multi-phase particle-in-cell (MP-PIC) methodology and the dense discrete phase model (DDPM) are also used to model flow behavior of particles. In MP-PIC particles with same properties are grouped into parcels and the collisions between these parcels are modeled by an ad-hoc solid stress term in order to reduce the high computational costs in treating a large number of particles [33–34], whereas the DDPM approach uses the kinetic theory of granular flow for calculating interactions between particles [35]. Thus, the MP-PIC and DDPM approaches do not solve the contact interaction for individual particles. Fundamentally, DEM solves Newton's equations of motion to resolve particle motion and uses a contact law to resolve inter-particle contact forces. Forces are integrated explicitly in time to predict the time history response of interactions of particles. The Hertz's theory of elastic contacts provides compact relations for the normal direction, derived from integration of the normal pressure distribution over the contact area [36]. A non-linear model, combining Hertz's theory is employed in modeling the contact between particles [37–38]. The elastic-plastic contact model provides energy dissipation through the irreversible plastic deformation after the yield initiation. Thornton et al. [39] compiled a comprehensive review of all known elastic and inelastic DEM contact models. A detailed review on computational fluid dynamics (CFD) coupled with the discrete element method (CFD-DEM) is reviewed by Deen et al. [40], Tsuji [41] and Zhu et al. [42] for the study of gas–solid flows in fluidized beds without consideration of reactions. The main feature of CFD–DEM is that it can generate detailed particle-scale information, such as the trajectories, forces and impact velocity of individual particles, which is key to elucidating the mechanisms governing the complicated flow behavior in gas-solid fluidized beds.

For flow of gas phase and monodisperse particles in fluidized beds, the solid phase can be described by either Eulerian solids phase using Eulerian basic framework or the discrete particle phase using Lagrangian basic framework in two reference frameworks. It is natural to expect that Eulerian solids phase field and Lagrangian discrete particle field are related. A major challenge in describing gas-solid fluidized beds, therefore, is to establish the precise relationship between these two phases. In present study, the monodisperse particles are described by both Eulerian solids phase in the Eulerian framework and the discrete particle phase in the Lagrangian framework. A coupled Eulerian fluid phase-Eulerian solids phase-Lagrangian discrete particle phase (CEEL) hybrid model is developed for modeling gas phase and monodisperse particles in the bubbling fluidized beds, as shown in Fig. 1. The CEEL model is aiming to have all fields of continuous gas phase, continuum solids phase and the motion of discrete particles in the gas-solid fluidized bed. The basic idea of present model approach is to use the continuum approach to describe the hydrodynamics of gas phase and continuum solids phase and the discrete element model to simulate the movement of individual particles. To the best of our knowledge, it is the first time to use it for modeling gas-solids fluidized beds.

2. Mathematical description

For simplify, we assume the gas phase is a compressible fluid, and the solid phase is treated as both the Eulerian solids phase and the discrete particle phase with the identical, smooth and inelastic spheres. The models use the principle of mass conservation and momentum balance for each phase. Present CEEL model equations are shown in the following paragraphs.

2.1. Discrete particle phase model

The trajectory of the discrete particles through the fluid is calculated by a force balance, which is calculated from Newton's second law [36]. Each particle is represented in a Lagrangian frame of reference by linear