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Three-dimensional simulation of gas–solid–liquid flows using the DEM–VOF method

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HIGHLIGHTS

- A DEM–VOF coupling model is proposed for simulating gas–solid–liquid flows.
- This model can compute complex three-phase motion and liquid displacement effects.
- It can also simulate curved walls and moving boundaries with ease.
- It is validated with tests of three-phase water entry, dam break and rotating tank.
- Results agree well with analytical and experimental data for validation.

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ABSTRACT

Gas–solid–liquid flows are widely found in chemical engineering, e.g. the processes of mixing, wet ball milling, and screw kneading, for which the numerical modeling is now a pressing research topic to help improve the design and investigate operational conditions. On the other hand, computational challenges are posed for existing methods in modeling the interphase interactions and complex boundaries within such three-phase systems. In this paper, an Eulerian–Lagrangian numerical model, specifically the DEM–VOF method, is presented for three-dimensional simulations of gas–solid–liquid flows. The fluid motion is solved by using a computational fluid dynamics (CFD) based approach with gas–liquid interface capturing provided by the volume-of-fluid (VOF) method. The particle phase is tracked by the discrete element method (DEM) as discrete entities. The fluid–particle coupling is achieved by the volume-averaging technique wherein a well-established empirical closure is adopted for the description of hydrodynamic forces. Particularly, the modeling of arbitrary-shaped walls and moving boundaries is addressed via the introduction of signed distance function (SDF) representation and immersed boundary (IB) method, which was proved to be highly efficient for gas–solid–liquid systems interacting with complex geometries. Special attentions when computing fluid–particle interactions near those boundaries are raised and their treatments are also discussed. Various model verifications and validation tests are performed in this study to show the validity and capability of the DEM–VOF method. By comparing with analytical solutions and experimental data, we generally find good agreements from the simulation results, thereby highlighting its potential in accurately modeling complicated gas–solid–liquid flows. To the best of our knowledge, the proposed method is the first report that successfully couples the DEM to a VOF solver with non-trivial wall boundaries.

1. Introduction

Gas–solid–liquid flows are widely encountered in chemical engineering. In particular, the motivation for our research focus is the pressing requirement for modeling gas–solid–liquid flows in wet ball/beads milling systems. In these problems, the complicated phenomena will restrict the observation and insight that could be obtained with experimental approaches. On the other hand, one may rely on accurate numerical simulations from which useful information could be extracted to help improve the designing and operating procedures.

For gas–solid–liquid flow problems, the numerical challenges mainly arise from interactions among different phases. Basically, a typical gas–solid–liquid flow involves fluid–fluid interaction (evolving fluid interface), fluid–solid interaction (fluid–particle momentum exchange), and solid–solid interaction (particle–particle collision). In

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addition, the influence of arbitrary-shaped geometries and moving boundaries must be taken into consideration for practical simulations. Prior to a systematic approach to complete gas–solid–liquid problems, some fundamental techniques have been established to solve those sub-problems independently.

- Fluid–fluid interaction
  A variety of numerical models have been developed to describe the motion of two-phase flows separated by immiscible fluid interfaces, e.g. the volume-of-fluid (VOF) method (Gueyffier et al., 1999), the level set (LS) method (Sussman et al., 1994), the coupled LS and VOF (CLSVOF) method (Sussman and Puckett, 2000), the front-tracking (FT) method (Unverdi and Tryggvason, 1992) and the constrained interpolation profile (CIP) method (Yabe et al., 2001). Those interfacial models are known to have their own features and limitations, which has been discussed in the literatures.
- Solid–solid interaction
  The discrete element method (DEM) (Cundall and Strack, 1979) or the discrete particle model (DPM) is now a common practice to simulate powder and granular materials. Its numerical strategy by directly tracking distinct particle motion allows for specific particle properties and exact evaluation of solid forces.
- Interaction with arbitrary-shaped wall boundary
  The immersed boundary (IB) method (Fadlun et al., 2000; Kajishima et al., 2001; Peskin, 1977) can efficiently model complex geometries non-conforming to the fluid grids, which has greatly alleviated the time-consuming mesh generation and regridding procedures in traditional computational fluid dynamics (CFD) techniques. Recently, the author's group has proposed an arbitrary-shaped wall boundary model (Shigeto and Sakai, 2013) based on signed distance function (SDF) which can offer a unified wall boundary representation for both fluid and particle simulations.

When it comes to the numerical analysis of more complex, coupled gas–solid–liquid flow systems, two classes of approaches have been employed so far: the direct numerical simulation (DNS) and the local volume-averaging technique, of which the former intends to resolve microscopic flow behaviors and the latter mainly focuses on macroscopic average flow problems. As opposed to the DNS that requires fine grids to resolve all relevant flow structures, the volume-averaging approach is less computationally demanding and thus it could be an affordable and pragmatic choice for simulating large-scale systems. The volume-averaging approach has its theoretical origin in the famous two-fluid model (TFM) (Anderson and Jackson, 1967; Gidaspow, 1994), where the interaction between two distinct phases is calculated based on empirical correlations. The DEM–CFD method (Tsuji et al., 1993) is among the most popular and successful numerical techniques based on a volume-averaging approach. The discrete particle phase is simulated by DEM-type Lagrangian methods and the fluid phase is computed on Eulerian meshes by using CFD. Hence such a coupling method is said to be an Eulerian–Lagrangian methodology. Compared with traditional TFM Eulerian description, this combination can overcome the analytical and numerical difficulties when modeling dense solid beds. The DEM–CFD method is now widely used to simulate solid–gas and solid–liquid fluidization systems. Review of DEM–CFD simulations of fluidized beds could be found in Deen et al. (2007), Zhu et al. (2008, 2007).

Despite the successful application of the volume-averaging Eulerian–Lagrangian model to two-phase fluidization systems, its power is not fully explored for gas–solid–liquid three-phase flows. Zhang and Ahmadi (2005) performed 2D simulation of slurry bubble columns in which motions and trajectories of disperse phases (bubbles and particles) are calculated by Lagrangian analysis procedure. As a result, there arises a dependency on empirical closure model to define the fluid–bubble interaction. Wen et al. (2005) described an interesting approach to model large-scale three-phase fluidization systems by combining DEM for particle phase and TFM for bubbly flows, where liquid–bubble interaction still relies on constitutive correlations. The fluid–particle momentum exchange is seemingly not balanced as different drag closures have been adopted in continuum and disperse phases separately. Additionally, their formulation is provided for axisymmetric coordinate but the DEM particle model is ambiguous in that case.

Fan's group has contributed some important results to the simulation of three-phase fluidization systems with direct computation of bubble motions. In Li et al. (2001, 1999) and Zhang et al. (2000a, 2000b), the authors proposed a 2D method combining the VOF method and a hard-sphere DPM in which a special close-distance interaction (CDI) model is included in the particle–particle collision process. Unfortunately, their formulation of gas–solid–liquid fluidization suffers from an inconsistent fluid–particle interaction model, as pointed out by Kafui et al. (2002). Later in their 3D studies (Chen and Fan, 2004; Ge and Fan, 2006), the LS method is used instead of the VOF method for the interface description. A review of their studies on gas–liquid-solid fluidized beds and bubble formation from nozzle in three-phase system is given by Yang et al. (2007).

A combination of FT method and hard-sphere DPM has been proposed in Van Sint Annaland et al. (2005) to simulate bubble rising and particle entrainment. However their study is restricted to the case of dilute particle suspensions (up to maximum 4% solid volume fraction) where the influence to fluid phase is not appreciable. Can et al. (2013) incorporated distinct particle tracing into a commercial VOF package for simulation of microchannel flows. Although the fluid–particle interaction is considered to be balanced, the interactions among solid particles are not included in their implementation. In Washino et al. (2013) a DEM–CIP coupling method is developed to calculate liquid droplet impingement on powder bed. They described a sub-grid scale model for the capillary action when the fluid interface penetrates into the solid layer, and the authors argued that this modeling can compensate the overestimated pushing effect due to drag force during the granular wetting process.

As briefly reviewed above, previous studies are found within a rather limited scope. Many of them are simple DEM–CFD extensions to three-phase fluidization systems in dilute regime. Particularly, we wish to identify several points that may obstruct the application to real engineering problems. First of all, more or less flaws could be found in many models concerning the formulation of the fluid–particle interaction term. This problem exists especially for some relatively early attempts, e.g. the VOF-DPM method by Li et al. (1999). It is no coincidence that such a model fails to verify the momentum balance between continuum and disperse phases. Secondly, it is not clearly documented in the past how the free surface behaves in response to the particle motion. For example, in mixing processes involving water entry and exit of solids, common issues are to model the deformation of the free surface disturbed by particles and the water displacement of the solid phase, of which the former is mainly credited with the dynamic fluid–particle interaction and the latter corresponds to the overall volume conservation property of the numerical approach. These vital considerations are, however, incidentally lacking in previous studies. Therefore the applicability of existing models to recover the macroscopic behavior of gas–solid–liquid flows in such problems is unknown. Lastly, it is found that no general geometries other than a simple rectangular computational domain have ever been treated throughout our literature survey. This means that the existing models cannot simulate three-phase flows interacting with curved geometries or moving parts widely encountered in engineering applications. One must be aware that, there is no trivial solution to this point because the influence of general geometries is an