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Implementation and validation of a volume-of-fluid and discrete-element-method combined solver in OpenFOAM

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ABSTRACT

Numerous gas–liquid–solid flows exist in chemical engineering and metallurgical processes. Numerical modeling is an important topic that can be used to improve the design and investigate the operating conditions of these processes. The complicated interphase interaction within such three-phase systems, which include free surfaces and discrete phases, poses challenges in the existing methods. We implemented a volume-of-fluid (VOF) and discrete-element-method (DEM) combined solver, which should be useful for modeling the gas–liquid–solid systems, within the OpenFOAM framework. The Du Plessis and Masliyah drag force, added mass force, and capillary force were considered for fluid–particle coupling. The VOF–DEM solver was tested in three different cases, namely, particles in pure gas, particle collision in water, and gas–liquid–solid three-phase dam break. The results were validated against previous experiments and good agreement was obtained between the simulations and the experiments, which indicates the accuracy and suitability of this VOF–DEM solver for gas–liquid–solid systems.

Introduction

Numerous gas–liquid–solid flows exist in industrial operations, such as in wet ball milling, ladle metallurgy and other chemical processes. For several decades, numerical models have gained considerable attention to investigate fluid–particle flows, especially in gas–solid systems, e.g., in fluidized beds and pneumatic conveying. Significant progress has been made to model systems with single fluid and solid particles (Alobaid & Epple, 2013; Cundall & Strack, 1979; Deen, Annaland, van der Hoef, & Kuipers, 2007; Huang, 2011; Luo, Wang, Yang, Hu, & Fan, 2017; Tsuji, Tanaka, & Ishida, 1992; Wang, Lu, Zhang, Shi, & Li, 2010; Xu & Yu, 1997), especially for gas–solid systems. Among the simulation approaches for such systems, the two-fluid model (TFM) (Anderson & Jackson, 1967) and the discrete element method (DEM) (Cundall & Strack, 1979; Tsuji et al., 1992) are the two most well-known methods. These approaches have been implemented in OpenFOAM (The OpenFOAM Foundation, 2014a, 2014b), which can refer to the solvers of TwoPhaseEulerFoam and DPMFoam. Thus far, except for the multi-fluid solver, there is no suitable solver with the particle behavior fully resolved for gas–liquid–solid three-phase systems in OpenFOAM.

An easy way to treat phases in gas–liquid–solid three-phase systems is in a uniform Eulerian coordinate, which is less computationally demanding, and so, it is useful in large-scale systems (Li & Zhong, 2015; Panneerselvam, Savithri, & Surender, 2009). The volume of fluid (VOF) and DEM combined method, which is considered an effective solution for gas–liquid–solid systems, was proposed by Li, Zhang, and Fan (1999) and Zhang, Li, and Fan (2000a, 2000b) in two dimensions. Chen and Fan (2004) and Van Sint Annaland, Deen, and Kuipers (2005) extended this approach to three dimensions by combining a front-tracking method and the DEM. Recently, other interface tracking approaches have been carried out combined with the DEM. Washino, Tan, Hounslow, and Salman (2013) presented a coupling of the DEM and a constrained interpolation profile to simulate the nucleation process in wet granulation. Sun et al. (Sun, Sakai, Sakai, & Yamada, 2014; Sun & Sakai, 2015) proposed two approaches by combining the moving particle semi-implicit (MPS) or VOF method with the DEM to simulate liquid–solid flows that involve free surfaces. The MPS (Koshizuka & Oka, 1996) can be used to deal with free surfaces based on Lagrangian particle methods that are similar to the smoothed particle hydrodynamics (SPH) (Monaghan, 1988). Within the context of Lagrangian methods, although the advection, deformation and topological change of the fluid interface can be simplified, one drawback is the need

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for large numbers of particles to produce simulations of equivalent resolution.

The motivation for this work is the implementation of a VOF–DEM combined solver in OpenFOAM, which is the most popular open-source computational fluid dynamics (CFD) code in academia and in industry. OpenFOAM version 3.0.0 was used and the developed solver is termed interDPMFoam. The fluid interface was solved by using the VOF method with considering the particle volume fraction, whereas the particle trajectory was calculated by using Newton's second law. The particle–particle or particle–wall interactions were resolved directly by using the DEM. For fluid–particle coupling, the Du Plessis and Masliyah (1991) drag relationship, which was proposed originally for total porosities in fluid–solid systems, was used. To consider the capillary force that was induced by the gas–liquid interface, an additional interfacial force was incorporated into the solver. Different cases were studied and the results were compared with experiments to test the new solver, and to determine its adequacy and suitability for simulations of gas–liquid–solid three-phase flows.

Model description

Volume-of-fluid method

The interface-tracking algorithm is based on the VOF method by solving a single set of momentum equations and by tracking the volume fraction of the liquid phase. OpenFOAM uses an improved version of the compressive interface-capturing scheme for arbitrary meshes (CICSAM) from Ubbink's work (Ubbink, 1997), in which a supplementary interface-compression velocity $\mathbf{u}_c$ is defined in the vicinity of the interface to steepen the gradient of the volume fraction and to improve the interface resolution. The conservation equation for the liquid volume fraction (γ) is solved in the following form:

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot (\gamma \mathbf{u}) + \nabla \cdot (\mathbf{u}_c \gamma (1-\gamma)) = 0, \tag{1}$$

where the compression velocity is calculated as (Weller, 2008):

$$\mathbf{u}_c = \min\left(C_\gamma |\mathbf{u}|, \max(|\mathbf{u}|)\right) \frac{\nabla \gamma}{|\nabla \gamma|}, \tag{2}$$

where C_γ is a constant that is used to control the intensity of compression. The momentum equation for the gas–liquid mixture is solved in the following form:

$$\rho\left(\frac{\partial(\varepsilon \mathbf{u})}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u}\mathbf{u})\right) = \varepsilon\left(-\nabla P + \nabla \cdot \left(\mu\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\right) + \rho \mathbf{g}\right) + \mathbf{F}_s + \mathbf{F}_p, \tag{3}$$

where ρ and μ are the density and viscosity of the mixture that are defined as:

$$\rho = \gamma \rho_l + (1-\gamma)\rho_g, \tag{4}$$

$$\mu = \gamma \mu_l + (1-\gamma)\mu_g, \tag{5}$$

ε is the void fraction in an Eulerian cell, which is calculated as:

$$\varepsilon = \max\left(1 - \frac{1}{V_{cell}} \sum_{\forall p \in cell} f_p V_p, \varepsilon_{min}\right), \tag{6}$$

where V_{cell} and V_p are the cell and particle volume, respectively, and f_p is the fractional volume of a particle that resides in a cell under consideration. ε_{min} is a value that is set to be slightly larger than 0 to avoid the cell from being occupied fully by a particle.

The surface tension is evaluated per unit volume by using the continuum-surface-force model (Brackbill, Kothe, & Zemach, 1992):

$$\mathbf{F}_s = \sigma \kappa \nabla \gamma, \tag{7}$$

where σ is the surface-tension coefficient and the curvature κ of the free surface is calculated as:

$$\kappa = -\nabla \cdot \left(\nabla \gamma / |\nabla \gamma|\right). \tag{8}$$

Discrete-element model

The translational and rotational motions of each individual particle with mass m_p are calculated from Newton's second law:

$$m_p \frac{d\mathbf{u}_p}{dt} = m_p \mathbf{g}\left(1 - \frac{\rho}{\rho_p}\right) + \mathbf{F}_c + \mathbf{F}_p, \tag{9}$$

$$I_p \frac{d\boldsymbol{\omega}_p}{dt} = \mathbf{T}_p, \tag{10}$$

where I_p is the moment of inertia, which is equal to $2m_p R_p^2/5$; $\boldsymbol{\omega}_p$ is the rotational velocity, and $\mathbf{T}_p$ represents the torque that is caused by the contact force. The particle–particle or particle–wall contact force $\mathbf{F}_c$ is determined from their overlap during a finite collision time and is calculated according to the model as proposed by Cundall and Strack (1979), which consists of a spring, a dash-pot and a slider, and the Hertzian spring-dashpot model is used. Details on the contact force and the determination of parameters can be found in Tsuji et al. (1992) and Li, Li, and Liu (2017).

Fluid–particle coupling

A two-way coupling is achieved via the sink term $\mathbf{F}_p$, which represents the momentum exchange between fluid and particles, such as drag force, virtual mass force, and Basset force. The drag force is written as:

$$\mathbf{F}_d = \frac{V_p \beta}{1-\varepsilon}\left(\mathbf{u} - \mathbf{u}_p\right), \tag{11}$$

where β represents the interphase momentum transfer coefficient from drag. Several drag relationships exist and details can be found in Li et al. (2017). In this work, a continuous relationship with the change in porosity as proposed by Du Plessis and Masliyah (1991), which is suitable for gas and liquid is used:

$$\beta = A\frac{(1-\varepsilon)^2}{\varepsilon}\frac{\mu}{d_p^2} + B(1-\varepsilon)\frac{\rho}{d_p}|\mathbf{u} - \mathbf{u}_p|, \tag{12}$$

where the coefficients A and B are given as:

$$A = \frac{26.8\varepsilon^3}{(1-\varepsilon)^{2/3}\left(1-(1-\varepsilon)^{1/3}\right)\left(1-(1-\varepsilon)^{2/3}\right)^2}, \tag{13}$$

$$B = \frac{\varepsilon^2}{\left(1-(1-\varepsilon)^{2/3}\right)^2}. \tag{14}$$

As indicated by several researchers (Huang, 2011; Li et al., 1999; Zhang et al., 2000a, 2000b), the added mass force has an important effect on particles in liquid. In this work, we consider the added mass force for fluid–particle coupling, which is written as:

$$\mathbf{F}_{am} = 0.5 V_p \rho \frac{d\left(\mathbf{u} - \mathbf{u}_p\right)}{dt}. \tag{15}$$

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