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Numerical study of coalescence and breakup in a bubble column using a hybrid volume of fluid and discrete bubble model approach

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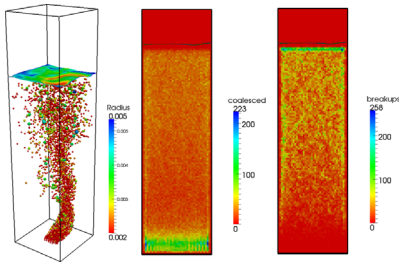
HIGHLIGHTS

- Modeling of free surface in bubble column is done using hybrid VOF-DBM approach.
- Free surface dynamics is captured in great detail in the model.
- Numerical parameters are tuned using experimental data from previous studies.
- A coalescence calibration factor and a critical Weber number are suggested using the study.

GRAPHICAL ABSTRACT



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ABSTRACT

In this work, two powerful methods are combined for bubble column simulations namely, the volume of fluid and the discrete bubble model. While the former method takes care of the free surface, the discrete bubble model tracks and handles the dynamics of the dispersed bubbles. The hybrid model presented in this work is verified and validated with existing established experimental results. A model parameter study for bubble break-up and coalescence is performed to find the optimum values of the model parameters, i.e. the critical Weber number and the coalescence calibration factor.

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1. Introduction

Bubbly flows are encountered in a variety of industrial applications. The majority of these flows entails a free surface, through which the bubbles leave the liquid. Experimental investigations of bubbly flows are difficult: the dynamic nature of the bubbly flow requires dynamic techniques that ideally do not disturb the flow. Moreover, for large systems one can either only measure macroscopic parameters like overall gas holdup or one is practically limited to measurements at a finite number of sample points. For such circumstances, computational fluid dynamics (CFD) has proven to be useful to extend the understanding of these flows, and to provide detailed information, both in space and time.

Several types of CFD models, dedicated to different length and time scales have been developed in the past few decades. Some authors adopt a multi-scale approach to understand and model large scale systems (Deen et al., 2004; Van der Hoef et al., 2004; Deen et al., 2007). In this approach, fully resolved simulations, also known as direct numerical simulation (DNS), are performed to obtain the micro-scale data. Through DNS studies, closures for various kinds of forces and coefficients are obtained, which can be used in coarse grained models like Euler–Lagrange models or

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two-fluid models (TFM). Usually, Euler–Lagrange models are employed for lab-scale simulations, while the TFM can be extended to industrial scale too. The advantage of using the former over TFM is that it provides details of bubble population in these bubbly flows, e.g. bubble size distributions are a direct result of the simulation.

Euler–Lagrange models usually treat the gas–liquid interface at the top of the column via some artificial boundary condition or a buffer zone technique (Streett and Macaraeg, 1989; Thompson, 1990; Poinsot and Lele, 1992; Pruett et al., 1995). The downsides of such boundary treatment are that (i) unphysical liquid circulation over the top surface can arise, and (ii) the dynamics of the free surface is ignored. In this study, an attempt has been made to formulate a numerical model introducing the free surface at the top of the column in the Euler–Lagrange framework. The model presented here combines the volume of fluid (VOF) model of van Sint Annaland et al. (2005) and the discrete bubble model (DBM) of Darmana et al. (2005). The hybrid model uses DBM to study the bubble and fluid dynamics in the bubble column, and the volume of fluid method to treat the free surface. Such a model formulation takes care of all the three phases, namely the liquid, the bubble and the gas phase. It is noted here that the bubbles are represented as dispersed elements, while the gas is treated as a continuous phase.

Volume of Fluid (VOF) methods (Hirt and Nichols, 1981; Youngs, 1982) employ a color function $F(x,y,z,t)$ that indicates the fractional amount of fluid present at a certain position (x,y,z) at time t. The advection equation for F is usually solved using a geometrical advection scheme, in order to minimize numerical diffusion. In addition to the value of the color function, the interface orientation needs to be determined, which follows from the gradient of the color function. The VOF technique in this work uses the piecewise linear interface calculation (PLIC) method of Youngs (1982) to reconstruct the interface.

In the discrete bubble model or Euler–Lagrange model, one phase (fluid) is solved on a Eulerian grid, while the other phase (bubbles, drops, particles etc.) is solved using the Lagrangian approach. The DBM accounts for bubble–liquid and bubble–bubble interaction using two way fluid–bubble coupling and a hard sphere collision model by Hoomans et al. (1996). In the current implementation, the bubbles are removed from the simulations domain as they reach the gas–liquid free surface.

Attempts have been made in the past to formulate models that combine interface tracking with bubble/particle/drop tracking. Tomiyama and Shimada (2001) have proposed a NP2 model, where they have combined the multi-fluid model with an interface tracking scheme. In the NP2 model, all the phases are solved in the Eulerian domain. Many authors have combined the discrete phase approach with the interface tracking, using CFD packages like Fluent and OpenFoam (Cloete et al., 2009; Mahrla and Hinrichsen, 2012; van Vliet et al., 2013). However, the basic disadvantage associated with these models is that the volume fraction of bubbles/particles is not considered while solving for the fluid-phase mass and momentum conservation equations. In dense bubbly flows, the volume fraction of bubbles should be accounted for in these equations. Therefore models excluding this aspect are valid only for dilute flows and should not be extended for studying systems with high volume fractions of the discrete phase. The model presented here overcomes the aforementioned shortcoming and will allow us to study dense bubbly flows with a free surface.

The organization of this paper is as follows: first the description of the model and the numerical solution method is given. Subsequently, numerical verification and experimental validation of the method is provided, where the simulated test cases are examined against the experimental findings from Deen et al. (2001). In the next section, a numerical parameter study of coalescence and breakup parameters is presented and discussed; and finally, the conclusions are presented.

2. Governing equations

Our model consists of two main parts: one part accounts for the presence of the gas–liquid free surface (VOF model) whereas the other part accounts for the presence of the bubbles in the liquid, taking into consideration the possible collisions between the bubbles themselves and/or confining walls (DBM). First, the main conservation equations are presented along with the incorporation of surface tension and the advection of the deformable interfaces. The fluid–bubble coupling and the bubble dynamics are subsequently described.

2.1. Mass and momentum conservation

The mass conservation equation for the fluid phase is described through the continuity equation:

$$\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot (\varepsilon_f \boldsymbol{u}_f) = 0 \tag{1}$$

where ε, and $\boldsymbol{u}$ represent the volume fraction and velocity, respectively. The subscript f refers to the fluid phase. The fluid phase includes both the liquid (l) and the gas (g) phases.

The momentum conservation can be described by the volume-averaged Navier–Stokes equations:

$$\rho_f \left[\frac{\partial (\varepsilon_f \boldsymbol{u}_f)}{\partial t} + \nabla \cdot (\varepsilon_f \boldsymbol{u}_f \boldsymbol{u}_f) \right] = -\varepsilon_f \nabla p - \nabla \cdot (\varepsilon_f \boldsymbol{\tau}_f) + \rho_f \varepsilon_f \boldsymbol{g} - \boldsymbol{f}_\sigma - \boldsymbol{f}_{l \to b} \tag{2}$$

where $\boldsymbol{f}_\sigma$ is the surface tension term, and $\boldsymbol{f}_{l \to b}$ is the forcing term for bubble–liquid interactions. Here the subscript b represents the bubble phase. Note that when $\varepsilon_f = 1$, the single phase Navier–Stokes equations are retained.

2.2. Volume of fluid approach

The volume of fluid approach uses the fractional amount of liquid to determine the interface position and orientation in a given cell. This fractional amount of liquid is often called the color function and is denoted by F.

$$F = \frac{\varepsilon_l}{(\varepsilon_l + \varepsilon_g)} = \frac{\varepsilon_l}{\varepsilon_f} \tag{3}$$

The liquid and the continuous gas together are regarded as the fluid phase (ε_f), the motion of which is described with an advection equation:

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + \boldsymbol{u}_f \cdot \nabla F = 0 \tag{4}$$

The fluid phase density is defined as

$$\rho_f = F\rho_l + (1-F)\rho_g \tag{5}$$

The local average fluid viscosity is calculated using a more fundamental approach proposed by Prosperetti (2002), via harmonic averaging of the kinematic viscosity of the involved phases according to the following expression:

$$\frac{\rho_f}{\mu_f} = F\frac{\rho_l}{\mu_l} + (1-F)\frac{\rho_g}{\mu_g} \tag{6}$$

2.2.1. Surface tension model

Among the surface tension models present, a recent publication by Baltussen et al. (2014) proposed a model for highly curved

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