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CFD-VOF-DPM simulations of bubble rising and coalescence in low hold-up particle-liquid suspension systems

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ABSTRACT

A combined CFD–VOF–DPM method has been used to simulate bubble rising and coalescence phenomenon in low hold-upparticle–liquid suspension systems. The liquid is considered as the primary phase, while particles are considered as the discrete phase. Bubbles or bubble parcels are regarded as the gas phase modeled using the VOF method. On the basis of the independence analysis of grid and time-step sizes, the combined method predicts fluid dynamics accurately with slight discrepancy according to the validation with experimental results. Subsequently, three-phase hydrodynamics are systematically investigated and thoroughly discussed.

1. Introduction

Bubbly flow has been frequently encountered in mixing and transport processes in multiphase reactors that play important roles in various industrial processes, such as direct coal liquefaction, Fischer–Tropsch synthesis, biomass liquefaction, and petroleum refinement [1]. A number of works have focused on bubbly flow reactors, and most of them were conducted as cold-model experiments (that is, processes at ambient temperature and atmospheric pressure without any reactions) [2–7]. With considerable improvement in computer algorithm and hardware, computational fluid dynamics (CFD) [8–16] has emerged as an effective and promising tool in studying the mesoscale and microscale flow structures inside bubbly flow reactors under harsh conditions (such as elevated temperature and pressure), which can be costly to investigate when conducted with experiments [17, 18].

Matters inside a reactor can be typically classified as continuous and discrete phases. When modeling the continuous phase with numerical tools, the Eulerian framework is mostly adopted. Meanwhile, when modeling the discrete phase, both Eulerian and Lagrangian frameworks are used as alternatives in previous studies [1, 8, 10, 13, 19–22]. The advantage of the Eulerian method is that it can provide macroscale average hydrodynamics properties that are of practical values. However, the Eulerian method requires constitutive equations for a closure model. From this point, the Lagrangian method requires few closure equations and can provide mesoscopic and even microscopic properties. Direct numerical simulation (DNS) method was adopted to capture the microstructure and interaction between continuous and discrete phases [23–25]. However, the required computational resource can be unreachable for DNS method. Hence, discrete particle method (DPM), which is based on the Lagrangian framework, is adopted to trace particle motion. On the basis of soft sphere model, researchers also considered particle–particle collisions [26]. To predict interfacial structure, researchers classified commonly adopted approaches as front tracking (such as maker-and-cell and immersed methods) and front capturing methods (e.g., level set, volume of fluid (VOF), and maker density function methods), which pertain to the fixed grid model [27, 28]. Among these interface tracking approaches, the VOF method is the most commonly applied method because of its stability and reliability in modeling interface topology changes. Hence, the VOF method is adopted in the present study [29–35].

Numerous outstanding studies were conducted for bubbly flow characterization. For gas–liquidtwo-phase flow, interaction and hydrodynamics were thoroughly investigated through not only using the Euler–Euler method but also the Euler–Lagrange method [1, 8, 11, 13, 19, 22, 36]. However, because of the complex interaction between phases (such as gas–liquid interaction, gas–solid interaction, liquid–solid interaction, and solid–solid collision), the understanding of three-phase bubbly flow is insufficient for gas–liquid–solid three-phase flow and thus needs further attention [33, 37–41]. Bubble hydrodynamics in three-phase flow has garnered considerable attention because of its violent mixing with liquid and solid (mostly particle) phases. According to experimental observation, bubbles typically undergo a series of stages, including bubble formation, rise-up, coalescence, and breakage. Numerous CFD simulations have reapplied this process perfectly [33, 39, 40, 42,43]. According to the literature, the properties of phase

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materials (such as density, viscosity, and surface tension) and operating conditions (including operating temperature and pressure) significantly influence bubble behavior. For instance, bubble size decreases with the increase in gas density when formed from an orifice; in addition, elevated pressures yield small maximum terminal bubble size [32, 44]. Despite being limitedly mentioned in previous studies, reactor size is another important parameter that influences bubble behavior [33]. Bubble behavior in pure liquid, especially bubble coalescence and breakage, is notably different from that in systems with particle phase or solid obstacle [45, 46]. However, to our best knowledge, no reports have emphasized bubble coalescence or breakage in the presence of particles. For solid-phasehydrodynamics, particle entrainment behind a rising gas bubble is believed as a salient phenomenon for gas–liquid–particle three-phase flow. This entrainment can induce wastage of catalyst particles or raw material particles and was qualitatively and quantitatively studied by few research groups via the Euler method or DPM [40, 42]. For liquid hydrodynamics, radial and axial liquid velocity profiles are strongly affected by bubble behavior, which are indispensable for understanding fluid dynamic performance in a bubbly reactor [33, 39, 40, 44].

In summary, researchers adopted specific multiscale models to simulate fluid characteristics under related time and length scales (Fig. 1) [37]. On the basis of a thorough understanding of the gas–liquid bubbly flow, we studied three-phase bubbly flow hydrodynamics. The objective of this work is to investigate a gas–liquid–solid three-phase flow system with low hold-up of particle concentration. To our best knowledge, this study is the first to investigate bubble rising and coalescence for three-phase systems. This remaining parts of the paper are organized as follows: first, the combined CFD–VOF–DPM model and the related cluster equations are described (Section2); subsequently, the simulation condition and strategy are determined and proposed (Section3); then, compelling results are presented and discussed (Section4); finally, the conclusions are drawn (Section5).

2. Models

Bubbles or bubble parcels are regarded as the gas phase in the present work. These forms are modeled using VOF method [33, 34, 47]. The volume fraction continuity equation is given by:

$$\frac{1}{\rho_q}\left[\frac{\partial}{\partial t}\left(\alpha_q\rho_q\right)+\nabla\times\left(\alpha_q\rho_q\vec{u}_q\right)\right]=0 \tag{1}$$

where ρ_q, α_q, and $\vec{u}_q$ respectively represent the density, volume fraction, and velocity of the qth phase. The primary-phase volume fraction will be computed based on the following equation:

$$\sum_{q=1}^{n}\alpha_q=1 \tag{2}$$

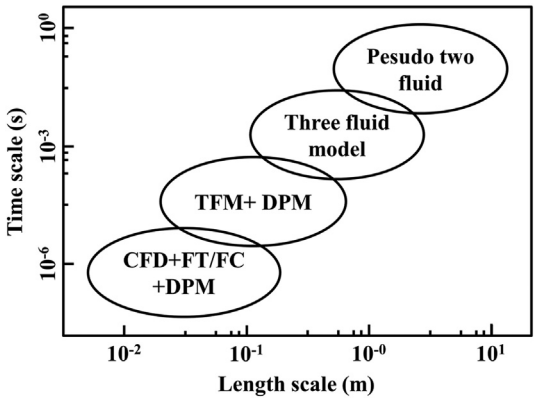

Fig.1. Four common multi-scale models for the three phase bubbly flow in this work.

the momentum equation is solved throughout the domain and shared by all the phases, which can be written as follows:

$$\frac{\partial\left(\rho\vec{u}\right)}{\partial t}+\nabla\cdot\left(\vec{u}\,\vec{u}\right)=-\nabla p+\nabla\cdot\left\{\mu\left[\nabla\vec{u}+\left(\nabla\vec{u}\right)^T\right]\right\}+F_{bp}+\rho\vec{g} \tag{3}$$

where ρ represents the density, $\vec{u}$ represents the velocity vector comprised of u_x and u_y in 2D (Cartesian coordinate system), μ represents viscosity, and $\vec{g}$ represents the gravitational acceleration vector with magnitude of g_x being zero and g_y of 9.81 m/s^2. F_{bp} represents the phase interaction forces from bubbles and particles, which can be expressed as follows:

$$F_{bp}=F_b+F_p \tag{4}$$

where F_p represents particle–liquid interface coupling relations derived from Newton's third law, and F_b represents bubble–liquid interface coupling interactions derived from the continuum surface force (CSF) model [48], which can be expressed as follows:

$$F_b=\sigma\frac{\rho\kappa\nabla\alpha}{0.5\left(\rho_g+\rho_l\right)} \tag{5}$$

where σ represents surface tension force and κ represents the free surface curvature, which is given by the following equation:

$$\kappa=-\left(\nabla\cdot\hat{n}\right)=\frac{1}{|\vec{n}|}\left[\left(\frac{\vec{n}}{|\vec{n}|}\cdot\nabla\right)|\vec{n}|-\left(\nabla\cdot\vec{n}\right)\right] \tag{6}$$

Moreover, the normal unit vector is defined as follows:

$$\hat{n}=\frac{n}{|n|} \tag{7}$$

The value of n was obtained from the following equation:

$$n=\nabla\alpha \tag{8}$$

The density and viscosity of the mixture in this work obey the mixing rule as follows:

$$\rho=\alpha\cdot\rho_l+(1-\alpha)\cdot\rho_g \tag{9}$$

$$\mu=\alpha\cdot\mu_l+(1-\alpha)\cdot\mu_g \tag{10}$$

The governing equations for solid phase are based on the Lagrangian framework. Particle motion can be typically divided into two modes, namely, translation and rotation. According to the Newton second law, ordinary differential equations that determine translational motion of particles can be written as follows:

$$\frac{dx_p}{dt}=\vec{u}_p \tag{11}$$

$$\frac{du_p}{dt}=F_D\left(\vec{u}-\vec{u}_p\right)+\frac{\vec{g}\left(\rho_p-\rho\right)}{\rho_p}+\vec{F}_c \tag{12}$$

where x_p is particle displacement, u_p is the particle velocity as a consequence of total volume force, $F_D(\vec{u}-\vec{u}_p)$ is the particle–liquid drag force, $\vec{g}$ is the gravitational acceleration vector with its components of $g_x=0$ and g_y=9.81 m/s^2, ρ_p and ρ are densities for particle and liquid, respectively, and $\vec{F}_c$ represents particle–particle collision force.

The interphase coupling relationships are shown in Eq. 12. The term of $\vec{g}(\rho_p-\rho)/\rho_p$ represents the sum of gravity and buoyancy forces, and