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Two-dimensional volume of fluid simulation studies on single bubble formation and dynamics in bubble columns

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ABSTRACT

In this paper, the volume of fluid (VOF) model in conjunction with continuum surface force (CSF) model was used to numerically investigate the single bubble formation and dynamics in the bubble columns on the software platform of Fluent 6.3. A set of transient conservation equations of mass and momentum taking surface tension and gravitational force effects into consideration were solved by pressure implicit splitting operator (PISO) algorithm and a piecewise linear interface calculation (PLIC) was applied to characterize the behavior of gas–liquid interface movement in the VOF method. The simulation results of bubble formation and dynamics compare well with available literature results. The effects of physical properties including surface tension, liquid viscosity and density, gas or liquid operation conditions and orifice size on the single bubble generation, detachment, rising and coaxial bubble coalescence were systematically analyzed, and the effect of superficial liquid velocity on single bubble behavior was especially discussed. It is found that non-zero superficial liquid velocity enhances the bubble detachment, decreases the bubble size, and delays the coaxial bubble coalescence obviously. Increasing superficial liquid velocity largely raises the velocity of the leading bubble and enlarging orifice gas velocity mainly accelerates the second bubble of two coalescence bubbles.

1. Introduction

Gas–liquid bubble columns are commonly used as multiphase reactors in the chemical, biochemical, environmental engineering, etc., for their advantages such as high mass and heat transfer and effective inter-phase contact (Clift et al., 1978; Deckwer, 1992; Drahoš et al., 1992; Krishna et al., 1993; Liu et al., 2004; Kantarci et al., 2005; Kulkarni and Joshi, 2005; Yang et al., 2007a,b, 2010, 2011). The single bubble behavior plays an important role in determining the flow, mass and heat transfer characteristics in the bubble columns and fluidized beds since its generation and rise can stir up the liquid and intensify the inter-phase disturbance, which makes sufficient inter-phase contact and efficiency improvement of mass and heat transfer in the reactors (Fan, 1989; Fan and Tsuchiya, 1990; Li et al., 1999, 2001; Zhang et al., 2000; Liu and Hu, 2004; Kulkarni and Joshi, 2005; Yang et al., 2007a,b; Ruzicka et al., 2009a,b; Rabha and Buwa, 2010). Hence, the study on single bubble behavior is a vital issue and many experimental and theoretical investigations on the bubble formation from an orifice, bubble shape variation and bubble rise velocity have been done in the past years (Clift et al., 1978; Liu and Hu, 2004; Kulkarni and Joshi, 2005; Yang et al., 2007a,b; Ruzicka et al., 2009a,b; Rabha and Buwa, 2010a,b).

With the advancements in numerical technique and computing power, the computational fluid dynamics (CFD) becomes a very effective means for exploring the bubble behavior. Several numerical simulations of single bubble formation and dynamics in liquids have been conducted in recent years and most numerical simulations applied simple but powerful volume of fluid (VOF) model based on the concept of a fractional volume of fluid to treat the complicated gas–liquid interface in the geometry (Hirt and Nichols, 1981; Tomiyama et al., 1993a,b, 1994; Hong et al., 1996; Lin et al., 1996; Delnoij et al., 1997; Krishna and van Baten, 1999, 2001; Li et al., 1999, 2000, 2001; Krishna et al., 1999, 2000; Takada et al., 2000; Koebe et al., 2002; Valencia et al., 2002; Son, 2003; Dai et al., 2004; Deen et al., 2004; Dijkhuizen et al., 2005, 2010a,b,c; van Sint Annaland et al., 2005; Bothe et al., 2006; Gerlach et al., 2006, 2007; Kurtoglu and Lin, 2006; Buwa et al., 2007; Ohta et al., 2005, 2007; Yang et al., 2007a,b; Hua et al., 2008; Minsier et al., 2009; Rabha and Buwa, 2010a,b).

There are three basic approaches commonly employed in the CFD for the study of multiphase flows: Eulerian–Eulerian (E–E) method, Eulerian–Lagrangian (E–L) method and direct numerical simulation (DNS) method (Delnoij et al., 1997; Krishna and van Baten, 2001; Li et al., 1999, 2001; Yang et al., 2007a,b). Since the E–E model treats the gas bubble or particles as a pseudo-continuum phase and the E–L model treats the gas bubble as a non-deformable spherical particle, both of these models are inappropriate for describing deformable bubble behavior, and the DNS approach has become important in characterizing details of the complex

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multiphase flow field. In the DNS of multiphase flow problems, there are various methods available for predicting phase interface position and movement, including the moving-grid method, the grid-free method and the fixed-grid method. The fixed-grid method is the most frequently used due to its efficiency and relative ease in programming. The numerical techniques used to solve the moving interface problem with fixed, regular grids can be categorized by two basic approaches: the front tracking method (the first front tracking technique applied in DNS: the marker-and-cell (MAC) method (Harlow and Welch, 1965) and improved one (Unverdi and Tryggvason,1992)) and the front capturing method (Delnoij et al., 1997; Yang et al., 2007a,b). The front tracking method explicitly tracks the location of the interface by the advection of the Lagrangian markers on a fixed, regular grid. The front capturing method, on the other hand, is the Eulerian treatment of the interface, in which the moving interface is implicitly represented by a scalar–indicator function defined on a fixed, regular mesh point. The movement of the interface is captured by solving the advection equation of the scalar–indicator function. At every time step, the interface is generated by piecewise segments or patches reconstructed by this scalar function. In this method, the interfacial force, such as the surface tension force, is incorporated into the flow momentum equation as a source term using the continuum surface force (CSF) method (Brackbill et al., 1992). This technique includes the VOF method (Hirt and Nichols, 1981), the marker density function (MDF) (Kanai and Miyata, 1998), and the level-set method (Osher and Sethian, 1988). The VOF method is designed for two or more immiscible fluids where the position of the interface between the fluids is of interest (Hirt and Nichols, 1981; Delnoij et al., 1997; Li et al., 1999, 2001; Krishna and van Baten, 2001; Yang et al., 2007a,b; Hua et al., 2008; Park et al., 2009). It is noted that there is also a Lagrangian VOF model (van Wachem and Schouten, 2002).

The VOF method was applied to study the formation and dynamics of a single gas bubble in a quiescent liquid at atmospheric pressures (Tomiyama et al., 1993a,b, 1994; Lin et al., 1996; Delnoij et al., 1997; Krishna and van Baten, 1998, 1999, 2001; Krishna et al., 2000; Takada et al., 2000; Koebe et al., 2002; Valencia et al., 2002; Son, 2003; Dai et al., 2004; Dijkhuizen et al., 2005; van Sint Annaland et al., 2005; Bothe et al., 2006; Gerlach et al., 2006, 2007; Kurtoglu and Lin, 2006; Buwa et al., 2007; Ohta et al., 2005, 2007; Yang et al., 2007a,b; Chakraborty et al., 2009; Minsier et al., 2009; Rabha and Buwa, 2010a,b) or elevated pressures (Li et al., 2000), including in the gas–liquid–solid fluidization systems (Hong et al., 1996; Li et al., 1999, 2001; Zhang et al., 2000; Yang et al., 2007a,b). The numerical simulation of air bubble formation and rising behavior in water shows that the formation process is characterized by three distinct stages of expansion, detachment and deformation and the bubble rises in a spiral path or a zigzag path (Krishna and van Baten, 1999; Yang et al., 2007a,b). The computed 2-dimensional (2D) or 3-dimensional (3D) bubble shapes, terminal velocities, structure of the wake of a gas bubble rising in a quiescent liquid and the coalescence of two coaxial gas bubbles under wide ranges of Eotvos number and Morton number resembled the experimental observations (Tomiyama et al., 1993a,b, 1994; Lin et al., 1996; Hong et al., 1996; Krishna and van Baten, 1998, 1999, 2001; Takada et al., 2000; Krishna et al., 2000; Ruzicka et al., 2009a,b). The simulation provides the time-dependent flow field information around the bubble and the particle and it reveals the mechanisms of the bubble formation and the interactions among the gas, liquid and solid phases during the bubble–particle collision (Hong et al., 1996; Yang et al., 2007a,b). The simulation of single bubble rising characteristics in a bubble column under the high pressure condition confirms with the phenomena of higher pressure yielding a smaller maximum stable bubble size in a bubble column (Li et al., 2000). The 3D VOF method featuring an interface reconstruction technique based on piecewise linear interface representation and a 3D version of the CSF model can handle a large density and viscosity ratio and a large value of the surface tension. The calculated terminal Reynolds numbers and shapes of isolated gas bubbles rising in quiescent liquids agree with flow visualization (van Sint Annaland et al., 2005; Dijkhuizen et al., 2005). Recently, the VOF model was applied to simulate the compressible gas bubbles (Pianet et al., 2010), bubble dynamics in polymeric solution (Hassan et al., 2010) and ionic liquids (Wang et al., 2010).

The VOF method is more suitable for the simulation of gas–liquid interfaces with large deformations because of its inherent mass conservation property, its suitability for the problems where large surface topology changes occur and reduced computational costs. However, it is less accurate in interface calculations than the other methods like the level set (LS) method. The combined LS and VOF (CLSVOF) method combines the advantages of both the LS and the VOF method (Son, 2003; Ohta et al., 2005, 2007; Gerlach et al., 2006, 2007; Buwa et al., 2007). A CLSVOF method was applied to simulate the formation, detachment and bubble rise above the submerged orifice in axisymmetric coordinates under constant inflow conditions. The operating conditions of the formation process such as orifice flow rate, orifice radius and wettability of the orifice plate were investigated for the working fluids of air and water. The numerical results of the bubble shapes, the bubble volume and the transition from a single to a double periodic formation process agree well with the experimental data available in the literature (Buwa et al., 2007; Gerlach et al., 2007). A CLSVOF model was also used to compute the slow formation of a gas bubble at an underwater orifice and the bubble contours agree well with the analytical counterparts based on the Young–Laplace equation (Gerlach et al., 2006; Ohta et al., 2005, 2007). The VOF model can be applied to simulate the rise of single or multiple bubbles in sheared liquids (Bothe et al., 2006; Rabha and Buwa, 2010a, 2010b). It was also applied to simulated the gas–liquid two-phase flow membrane separation and membrane bioreactors (Taha and Cui, 2002; Ndinisa et al., 2005; Taha et al., 2006; Ratkovich et al., 2009; Buetehorn et al., 2011). The use of gas–liquid two-phase flow has been shown to significantly enhance the performance of some membrane processes by reducing concentration polarization and fouling. Taha and Cui (2002) used the 2D VOF method to calculate the shape and velocity of the slug, as well as the velocity distribution and local wall shear stress at the membrane surface in the upward slug flow ultrafiltration process to explain the mechanism of the permeate flux enhancement resulting from gas sparging in tubular membrane modules. Taha et al. (2006) employed the 3D VOF method to simulate the details of slug flow dynamics in horizontal and inclined gas-sparged ultrafiltration processes to identify the enhancement effect on ultrafiltration performance. Ndinisa et al. (2005) compared the performance of the 2D VOF model and two-fluid Eulerian model in simulating the Taylor bubbles in tubular membranes and found that the two-fluid Eulerian model showed a better performance than the VOF method on the basis of comprehensive comparison. Buetehorn et al. (2011) used VOF method to simulate the effect of hydrodynamic conditions on the performance of single- and, multiphase flows with submerged membrane bioreactors with irregular fiber arrangement and found that a proper Taylor bubble flow is developed before the bubble enters the porous medium. Ratkovich et al. (2009) employed a CFD model with the 2D VOF method to model the effect of slug flow on the surface shear stress in a vertical tubular membrane. The results indicated that the CFD model was able to accurately simulate shear stresses induced by gas slugs for conditions of high liquid and low gas flow rates.