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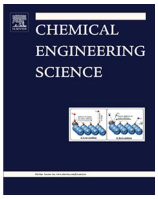

Numerical simulation of bubble formation with a moving contact line using Local Front Reconstruction Method

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HIGHLIGHTS

- A novel Local Front Reconstruction Method with contact line dynamics is presented.
- Two different methods to take into account the triple contact line are implemented.
- Model is verified and validated.
- Effect of the flow rate on the bubble formation is determined.

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ABSTRACT

The process of adiabatic bubble formation from an orifice plate occurs in various industrial applications. It is important to understand the dynamics of bubble formation and to develop numerical models to accurately predict the formation dynamics under various operating conditions. For the numerical models, an appropriate contact line boundary condition is necessary since this process may involve a moving contact line, which significantly affects the bubble departure size. In this paper, we extend the Local Front Reconstruction Method by incorporating contact angle dynamics. The predictions of the improved model are extensively verified and validated with experimental and numerical data available in the literature. The problem of three-dimensional bubble injection from an orifice into quiescent water using various volumetric flow rates is used to assess the numerical model under capillary dominant conditions and conditions where the interplay between inertial, viscous, surface tension, and buoyancy forces cause a complex interface deformation.

1. Introduction

The formation of gas bubbles by submerged needles or orifices is of great interest for diverse applications in chemical, nuclear, and metallurgical industries, because it influences the bubble size and thereby the bubble rise velocity. To optimize the bubble formation (e.g., the formation time, bubble volume and motion of the contact line), the fundamental physics should be understood. However, some of this fundamental knowledge is still lacking (Kulkarni and Joshi, 2005).

Several studies on the formation of bubbles have already been performed using both experimental and numerical approaches. The majority of these studies focused on the case of bubble formation using a constant volumetric gas flow rate through a submerged orifice (McCann and Prince, 1971; Zhang and Shoji, 2001; Badam et al., 2007; Das et al., 2011). Experimental and theoretical studies have shown that the forces acting on the bubble during the growth are divided into two main groups according to their influence on the formation. The first group causes the bubble detachment. This group includes the buoyancy, gas injection momentum, and contact pressure forces, which emerges due to the pressure difference inside and outside of the bubble over the contact area. The second group includes viscous, surface tension, and inertial forces. This group resists the bubble detachment and tends to keep the bubble attached to the orifice (Duhar and Colin, 2006; Di Bari and Robinson, 2013).

For single bubble growth at a constant gas flow rate, three formation regimes have been identified. The first regime is the static regime, which prevails at low gas flow rates. In this regime, there is equality between buoyancy and surface tension forces. The volume of the formed bubbles is independent of flow rate; decreasing the flow rate will increase the formation time. At higher flow rates, bubble formation enters the dynamic regime. Because the bubbling

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mode is more complicated, this regime is divided into six bubbling modes. Contrary to the static regime, the formation time is constant while the bubble volume is affected by the flow rate. The bubble evolution is governed by the interplay of inertial, viscous, surface tension, and buoyancy forces. Under even greater flow rates, bubble formation enters the turbulent regime. In this regime, successive bubbles coalesce with each other close to the orifice and they rise only a small distance above the orifice before they are shattered into many small bubbles of varying size by the strong turbulence (McCann and Prince, 1971).

Several phenomenological models were proposed to describe the bubble growth and detachment based on extensive experimental data sets. Earlier theoretical studies focused on the development of an analytical model to derive a scaling law for the volume of a detaching bubble assuming that the bubble retained a spherical shape (Davidson and Schüler, 1960a; Davidson and Schüler, 1960b; Kupferberg and Jameson, 1969; Gaddis and Vogelpohl, 1986). Marmur and Rubin (1976) proposed a more realistic mathematical model for non-spherical bubbles to predict the bubble volume by dividing the bubble interface into finite differential elements. In addition, a simple Young-Laplace equation could be used to describe the bubble motion at sufficiently low gas flow rates (Marmur and Rubin, 1973; Gerlach et al., 2005; Lesage et al., 2013; Lesage and Marois, 2013). Although these approaches are in good agreement with experiments in certain regimes, the majority of them are unable to account for the viscous effects, bubble interactions and the last phase of the neck pinch-off at detachment. More advanced mathematical models are necessary to accurately describe the whole parameter space of interest.

Due to the fast developments of the computational resources and numerical methods over the last decades, it is possible to conduct detailed Direct Numerical Simulations (DNS) of multiphase flows. These simulations are performed by either interface capturing methods or interface tracking methods, since moving grid methods are often limited to moderately deforming interfaces (Baltussen et al., 2014; Weber et al., 2017). Both interface capturing and interface tracking methods assume a one fluid approximation, whose properties are determined from the interface position. The essential difference between these methods is the interface treatment. In interface capturing methods, the interface is reconstructed from an indicator function, which is advected by the fluid velocity on a fixed Eulerian grid. The most widely used interface capturing approaches are the Volume of Fluid (VOF) method (Hirt and Nichols, 1981), the Level Set (LS) method (Osher and Sethian, 1988) and a combination of these two, known as Combined Level Set and Volume of Fluid (CLSVOF) method (Sussman and Puckett, 2000). All these three methods have been extensively used to study multiphase flows including bubble formation at an orifice (Valencia et al., 2002; Gerlach et al., 2007; Chakraborty et al., 2009, 2011; Ma et al., 2012; Yujie et al., 2012; Albadawi et al., 2013; Georgoulas et al., 2015). In the front-tracking methods, the motion of the interface can be captured more accurately because the method tracks the interface with separate Lagrangian interface elements, improving also the surface tension calculation (Unverdi and Tryggvason, 1992). In spite of its attractiveness, the original front-tracking method does not allow interface merging or breakup. Therefore, it cannot be applied for the simulation of bubble growth and detachment. Several authors have proposed new techniques that enable the front-tracking method to automatically and robustly model the merging and breakup of interfaces (Shin and Juric, 2002; De Sousa et al., 2004; Quan and Schmidt, 2007; Shin et al., 2011). In the present work, we have chosen a front-tracking algorithm that allows interface merging and breakup, the Local Front Reconstruction Method (LFRM) (Shin et al., 2011). The LFRM has been validated with several benchmarking tests and the results demonstrate excellent performance in maintaining detailed interfacial shapes and local mass conservation especially at low-resolution.

In many cases of formation of bubbles from an orifice plate, the bubbles are not pinned to the orifice rim. This movement of the contact line will introduce an extra aspect in the calculation, namely the wettability. When a bubble is formed on a thin-walled nozzle, the behavior of the moving contact line has little influence on the diameter of the detached bubble (Oguz and Prosperetti, 1993). However, when forming on an orifice plate, both the apparent contact angle and the contact line diameter vary as the bubble grows in size. Unfortunately, the experimental and numerical studies on the contact line behaviors during bubble formation are very limited and as far as the authors know no universal pattern of the time-history of the contact angle and contact diameter has been determined (Chigarev and Chigareva, 1986; Kandlikar and Steinke, 2002; Gnyloskurenko et al., 2003; Chen et al., 2013). Experiments show that for a hydrophilic surface, the contact line will not recede very far from the orifice, or it may even remain pinned to the orifice rim for the whole bubble formation process (Gnyloskurenko et al., 2003; Byakova et al., 2003). On the other hand, the contact line of a bubble forming on a hydrophobic surface will recede much further, thus increasing the formation time and the volume of the bubble formed (Gnyloskurenko et al., 2003).

The introduction of a moving contact line in the mathematical model results in a number of challenging issues. First of all, a complete mathematical representation of the motion of the triple contact line is still a problematic task. It is well known that the no-slip boundary condition yields stress singularity at the contact line since the fluid velocity is finite at the free surface but zero on the wall (Huh and Scriven, 1971). This singularity is usually removed by relaxing the no-slip boundary condition with a slip model. The most common approach is to use a relation between the apparent contact angle and a contact line velocity using a contact line model derived from theory (e.g. that of Cox, 1986; Blake, 2006; Kistler, 1993). The contact line position is then determined by specifying the apparent contact angle computed from the contact line model. Typically, no-slip boundary condition is still imposed on the wall for the fluid velocity since slip condition may lead to a singularity in the pressure (Sui et al., 2014). The velocity components tangential to the wall at the nearest grid node or marker point are then used as the contact line velocity (Francois and Shyy, 2003; Saha and Mitra, 2009; Yokoi et al., 2009; Muradoglu and Tasoglu, 2010). Although, the unresolved contact line region is somewhat large for DNS, Kafka and Dussan (1979) showed that for a nanometer slip length, an interfacial angle at a distance to the contact line ranging from $O(10\,\text{nm})$ to $O(10\,\mu\text{m})$ leads to no significant differences in the outer region.

Several attempts have been made to provide macroscopic models of the contact line dynamics based on the microscopic physics for droplet simulations (Sui et al., 2014). However, only a few numerical studies on bubble formation have taken into account the effects of moving contact line. The majority of the authors simulated the bubble formation process with the contact angle kept equal to the static contact angle (Higuera, 2005; Higuera and Medina, 2006; Gerlach et al., 2007). Chen et al. (2013) studied the contact line behaviors during bubble formation using two kinds of contact angle models in their LS method: a contact line velocity dependent model and a stick-slip model. They showed that the stick-slip model is more accurate in describing the contact line dynamics.

In the present work, we improve the 3D-LFRM by incorporating contact angle dynamics and apply the combined method to the simulations of bubble formation from submerged orifice. The paper is organized as follows: The numerical model is presented in Section 2. Section 3 presents the verification of the contact angle