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On the assessment of a VOF based compressive interface capturing scheme for the analysis of bubble impact on and bounce from a flat horizontal surface

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A B S T R A C T

The process of free rise, collision on and bounce from a solid horizontal surface for a single isolated bubble is investigated by numerical simulations based on the Volume of Fluid method (VOF). The volume fraction advection equation is solved algebraically using the compressive scheme implemented in the CFD open source library (OpenFOAM®) using both axi-symmetrical and three dimensional domains. The solution sensitivity to the mesh refinement towards the solid boundary and the contact angle formulation (static and dynamic) are assessed with two different fluid mixtures for a range of Bond numbers [0.298–1.48] and two different surface hydrophilicities. Numerical results are assessed against published as well as new experiments to include both axi-symmetrical and three dimensional rise trajectories. The investigation addresses the liquid microfilm formation and drainage considering both flow and pressure fields and bubble dynamic characteristics over successive rebounds. Results highlight the importance of resolving the liquid microlayer at the interface between the gas and solid surface in particular in the case of superhydrophobic surfaces. A coarse mesh is shown to precipitate the liquid film drainage. This results in early formation of a triple phase contact line (TPCL) which can occur as soon as the first rebound whereas physical observations indicate that this typically happens much later at a stage when a significant part of the bubble kinetic energy has been dissipated following several rebounds. As a result numerical predictions are shown to be much more sensitive to the contact angle formulation than when a refined mesh allows a more accurate representation of the film drainage. In this case, static and dynamic contact angle models give broadly similar rebound characteristics. Following validation, the numerical simulations are used to provide some useful insight in the mechanisms driving the film drainage and the gas liquid interface as it interacts with the solid surface.

1. Introduction

The flow of dispersed gas bubbles in liquid can induce localized and large scale mixing. Both can be exploited in industrial processes ranging from effective heat exchangers to bioreactor or filtration applications, just to name a few. The focus of the present study is on rising air bubbles colliding with a solid surface. Recent work has shown that the bubbles in such cases can induce very significant and sharp increases in convective cooling from the surface (Delauré et al., 2003; Donoghue et al., 2012). The two-fluid flow mechanisms involved present specific challenges which continue to make accurate experimental and numerical analysis particularly complex. A number of experimental and numerical investigations have been dedicated to the study of a single isolated bubble growing from a capillary or wall orifice (Di Bari and Robinson, 2013; Albadawi et al., 2012, 2013; Lesage et al., 2013) and rising freely in a bulk liquid [see Clift et al. (1978), Bhaga and Weber (1981) and most recently Legendre et al. (2012), Ohta and Sussman (2012), and Chakraborty et al. (2013)]. Much fewer experimental studies have considered the bubble's interaction with solid surfaces and, to the authors' knowledge, no published research has attempted to assess the accuracy of Volume of Fluid (VOF) methods for modeling the bubble bouncing in three dimensions.

The process of bubble impacting and bouncing on a horizontal plane following a phase of free rise can be characterized by three main stages, (i) the bubble deformation prior to impact or following rebound, (ii) the film formation and drainage in the intervening region between the bubble and the wall and (iii) the film rupture

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when the air in the bubble comes in direct contact with the solid surface. The mechanism of the bubble bouncing has tended to be categorized and studied to reflect the very different length scales involved at each stage, i.e. whether the interest is in the millimeter sized bubble, the microfilm, or the interface contact line in the inner region within a few nanometers of the wall. Published studies have considered the geometrical characteristics of the bubble shape during the full bouncing process, the film formation and drainage, and finally the three phase contact line (TPCL) formation and surface de-wetting which takes place at the moment when the film thickness becomes smaller than a specific limit.

In the first group, the bouncing process and the number of bouncing cycles have been analyzed based on the bubble initial kinetic energy before collision (Tsao and Koch, 1997; Zawala et al., 2007). The bubble behavior is typically described using geometrical characteristics such as the bubble center of gravity, aspect ratio, and coefficient of restitution (Legendre et al., 2005; Zenit and Legendre, 2009). Other experimental studies have focused on investigating the influence of the surfactant distribution in the bulk liquid (Malysa et al., 2005) and the surface material properties (Krasowska et al., 2009; Fujasova-Zednikova et al., 2010; Kosior et al., 2012). Studies in this group focus on the first stage of the collision when the bubble rebounds from the surface, and have not included studies of the film and TPCL formations.

In the second group, research has concentrated on the flow field in the film region. Studies have, to a large extent, relied on the lubrication theory to model the liquid film trapped between the bubbles and surfaces. Klaseboer et al. (2001) and Hendrix et al. (2012) followed this approach to study the film thinning process. Of interest to the present article is their conclusion on the development of a high pressure region and its importance as the main driving force in the bubble rebound. Chan et al. (2011) presented a review of experimental approaches developed for the study of the spatio-temporal evolution of the drainage of films forming between drops and flat surfaces, drops and particles and between drops. Numerically, the potential flow theory has also been adapted by Klaseboer et al. (2012) to account partially for viscosity effects with a solution based on a Boundary Element Method. Comparison of the rebound amplitudes with experimental results, however, showed that the method failed to account fully for energy damping.

At the last stage of bouncing when the film thickness decreases to the point where the drainage is controlled by intermolecular forces between the liquid/gas and solid molecules, the properties of the surface material influence the interface and bubble dynamics with either a contact line formation (for hydrophobic surfaces) or the stabilization of a permanent film between the bubble and the wall (for hydrophilic surfaces). Although the dynamic of wetting/de-wetting with the TPCL formation has been extensively studied [see the reviews by De Gennes, 1985; Shikhmurzaev, 1997; Bonn et al., 2009], the details of displacement of one fluid by another on a solid surface is still not well understood. In general, two different approaches have been adopted; the hydrodynamic model (Cox, 1986), and the molecular kinetic model (Blake and Haynes, 1969). De-wetting due to a small air bubble rising in deionized water and hitting a horizontal wall has been studied experimentally by Phan et al. (2006) and Fetzer and Ralston (2009). Both studies have focused on the last stage of the bouncing starting from the moment when the TPCL forms and did not extent to other stages of bouncing. Apart from this, most research on TPCL formation have considered drop impact rather than bubble bounce and all have highlighted parametric sensitivity of both hydrodynamic and the molecular kinetic models which are all based on some level of empiricism. To the author's knowledge, no published study have attempted to analyze and quantify this sensitivity when the hydrodynamic wetting dynamic model is coupled with a VOF model for the study of impacting and bouncing of air bubbles.

However, there has been an increasing focus on the numerical models for the bubble surface interactions in an effort to characterize the bubble geometrical characteristics and surrounding flow field during the film formation. Canot et al. (2003) managed to couple a Boundary Element Method with a lubrication approximation. This coupling made it possible to model the full dynamics of the bubble bouncing but did not consider a three-dimensional (3D) case. Differences in the energy of surface deformation meant that no quantitative comparison with experimental data could be done. The analysis of the bubble-wall collision dynamics and the corresponding energy dissipation have been studied by Omori et al. (2010) using a front tracking method (Muzaferija and Perić, 1997) for two-dimensional (2D) bubbles with two different equivalent diameters ($1, 2$ mm). The model was shown to correctly capture the thin liquid film and the formation of a characteristic dimple before rebound but no detail about the contact line model at rigid walls were provided. Sanada et al. (2005) solved the full Navier Stokes equations coupled with the Level Set method for the analysis of bubble bouncing against a free surface (air/water). Contrary to Tsao and Koch (1997), they found that when the bubble approaches the free surface, the pressure in the film does not increase strongly leading the author to suggest that the bouncing process is not entirely controlled by flow properties in the liquid film. Most recently, Qin et al. (2013) used an arbitrary-Lagrangian–Eulerian approach for the study of bubble-wall interaction at high Morton numbers. The flow field in the liquid domain was solved in this case using a Finite Element formulation while the flow in the gas domain was neglected. The bubble interface tracking relied on a moving mesh and the film drainage was simulated using an adaptive mesh to keep at least three cells in the region between the bubble surface and the wall. This meant that the film rupture could not be modeled so that simulation were stopped whenever the film thickness reaches a value $1/100$ of the bubble radius.

In spite of extensive numerical modeling work on dispersed gas bubble flows and on the dynamics of drops impinging upon solid surfaces [see for example Sikalo et al. (2005), Dupont and Legendre (2010)], there is still a distinct lack of understanding on the suitability of the commonly used VOF interface capturing method and some of the main contact line models to correctly capture the mechanisms of air bubble impacting on and bouncing from a surface. Its ability to model the correct spatio-temporal characteristics of the liquid film formation and drainage including pressure distribution and its effect on the bubble dynamics still needs to be studied. This is the focus of the present study. The 3D mechanisms of bubble bouncing (approach, collision, film formation, and contact line formation) on a horizontal surface is analyzed in the present study by solving the full Navier Stokes equations coupled with the compressive VOF method implemented in the open source solver library (OpenFOAM-2.1). The analysis aims to clarify the importance of the mesh resolution and its suitability to the contact line model by comparing modeled bubble and film characteristics with new and published experimental results. The analysis includes quantitative descriptions of (i) the film formation and variations in the film thickness (ii) the pressure distribution and flow velocity field in the film region to explain the damping reasons during the bouncing (iii) the influence of the contact line models on the bubble dynamics at the last stages of the bouncing process.

2. Mathematical formulation

2.1. Governing equations and computational method

The mass and momentum equations solved for this isothermal, incompressible and immiscible two phase flows have the following conservative form: