Accepted Manuscript

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PII: S0301-9322(14)00109-8

DOI: <http://dx.doi.org/10.1016/j.ijmultiphaseflow.2014.05.017>

Reference: IJMF 2055

To appear in: *International Journal of Multiphase Flow*

Received Date: 27 November 2013

Revised Date: 27 May 2014

Accepted Date: 28 May 2014

Please cite this article as: Albadawi, A., Donoghue, D.B., Robinson, A.J., Murray, D.B., Delauré, Y.M.C., 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, *International Journal of Multiphase Flow* (2014), doi: <http://dx.doi.org/10.1016/j.ijmultiphaseflow.2014.05.017>

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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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Abstract

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 micro layer 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

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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.

Keywords:

Gas-Liquid Flow; VOF method, Bubble bouncing; static and dynamic contact angle; mesh resolution; film drainage

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); 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 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:

$$\nabla \cdot \mathbf{V} = 0 \quad (1)$$

$$\frac{\partial(\rho \mathbf{V})}{\partial t} + \nabla \cdot (\rho \mathbf{V} \mathbf{V}) = -\nabla P + \nabla \cdot \tau + \rho \mathbf{g} + \mathbf{F}_\sigma \quad (2)$$

where ρ and μ are the fluid density and viscosity, $\mathbf{g}$ the gravitational acceleration, $\mathbf{V}$ the fluid velocity vector, τ the viscous stress tensor defined as $\tau = 2\mu S = \mu[(\nabla \mathbf{V}) + (\nabla \mathbf{V})^T]$, P the static pressure, and $\mathbf{F}_\sigma$ the volumetric surface tension force. The Volume of Fluid method implemented in the OpenFOAM-2.1 is used for capturing the interface. The fluid domain is modeled as a single mixture but a scalar function α is used to distinguish between the two fluids. α is defined as the volume fraction of liquid in each cell. It has a value of 0 in the gas phase and the value 1 in the liquid phase while the interface is defined as an α iso-contour in the range ($0 < \alpha < 1$). Because of the algebraic interface scheme, the interface is typically spread over 3 cells and generally not more than 5 cells. The physical properties of the mixture are also defined in terms of the volume fraction α as:

$$\rho = \rho_l \alpha + \rho_g (1 - \alpha) \quad (3)$$

$$\mu = \mu_l \alpha + \mu_g (1 - \alpha) \quad (4)$$

where the subscripts l and g stand for liquid and gas, respectively.

The modified pressure $P_{rgh} = P - \rho \mathbf{g} \cdot \mathbf{x}$, where $\mathbf{x}$ is the position vector, is used for the solution of the governing equations to avoid a steep change in the pressure across the bubble interface which would otherwise exist due to the large density difference. A cell centered finite volume formulation is used for the discretization with an implicit first order Euler scheme and second order schemes for the time and space discretization, respectively. The volumetric surface tension force is estimated in terms of the gradient of the volume fraction following the continuum surface force model (CSF) proposed by Brackbill et al. (1992) as:

$$\mathbf{F}_\sigma = \sigma \kappa(\alpha) \nabla \alpha \quad (5)$$

where σ is the surface tension coefficient and κ is the interface curvature which is calculated as:

$$\kappa = -\nabla \cdot \hat{\mathbf{n}}_c \quad (6)$$

161 where $\hat{\mathbf{n}}_c$ is the unit interface normal calculated using the phase fraction
162 field:

$$\hat{\mathbf{n}}_c = \frac{(\nabla\alpha)}{|\nabla\alpha|} \quad (7)$$

163 In the VOF method, the interface is tracked by solving the continuity
164 equation for the volume fraction which is defined as:

$$\frac{\partial\alpha}{\partial t} + \nabla \cdot (\mathbf{V}\alpha) + \nabla \cdot (\mathbf{V}_c\alpha\beta) = 0 \quad (8)$$

where $\beta = 1 - \alpha$. The compressive velocity ($\mathbf{V}_c$) is added to counter diffusion of α at the interface. It is defined in OpenFOAM as a function of the flow velocity magnitude and to point in direction perpendicular to the interface with:

$$\mathbf{V}_c = \min(c_\alpha|\mathbf{V}|, \max(|\mathbf{V}|)) \frac{\nabla\alpha}{|\nabla\alpha|} \quad (9)$$

165 A coefficient c_α greater than 1 can be used to increase compression of the
166 interface in which case the limiter ($\max|\mathbf{V}|$) defined as the largest value of
167 $|\mathbf{V}|$ over the full domain ensures that the global maximum velocity is not
168 exceeded. In this study, $c_\alpha = 1$ has been used so that Eq. 9 is equivalent to
169 $\mathbf{V}_c = |\mathbf{V}|(\nabla\alpha/|\nabla\alpha|)$. The interface compression is achieved by the scalar
170 multiplier $\alpha\beta = \alpha(1 - \alpha)$ which has a maximum of 0.25 at the interface and
171 tends to zero when α tends to 0 or 1, i.e. in the gas or liquid phase (Weller,
172 2008). The divergence in the compressive velocity in Eq. 8 is discretized
173 using the second order van Leer scheme (van Leer, 1979), while the last term
174 is discretized using the interface compression scheme proposed by Rusche
175 (2002). The Pressure Implicit with Splitting of Operators (PISO) algorithm
176 (Issa, 1986) was used for the pressure-velocity coupling (For more details on
177 these schemes see (OpenFOAM-2.1, 2013; Berberović et al., 2009; Albadawi
178 et al., 2013)).

179 2.2. Contact angle boundary condition

180 The contact line region is decomposed into two main parts; the outer
181 macroscopic region where inertia forces cannot be neglected and the inner
182 region where inertia has little influence (Bonn et al., 2009). The details of
183 the flow in the inner region can be simulated using a slip length of molecular
184 scale. Computational restrictions, however, means that in most practical
185 problems the very small scales involved cannot be resolved and molecular

forces are typically represented by a local force parallel to the wall. Surface tension is still evaluated from the CSF model but the interface normal used to evaluate the curvature is defined by Eq. 10 instead of Eq. 7.

$$\hat{\mathbf{n}} = \hat{\mathbf{n}}_w \cos \theta_i + \hat{\mathbf{t}}_w \sin \theta_i \quad (10)$$

where $\hat{\mathbf{n}}_w$ is the unit normal to the wall and $\hat{\mathbf{t}}_w$ is the unit vector located at the wall and normal to the contact line formed between the gas/liquid interface and the wall. This contact angle formulation is commonly used (see for example Sikalo et al. (2005)) and is adopted in the present study.

The imposed contact angle controls the interface slope in the matching area between the inner and the outer regions. By imposing a specific boundary contact angle, the interface curvature is changed and the surface tension force must adapt. In a static case the solution converges to an equilibrium state and the angle formed by the interface at the solid wall converges to the equilibrium contact angle (θ_e). Two different contact angle definitions may be used; (i) the static ($\theta_i = \theta_s$) and (ii) dynamic contact angles ($\theta_i = \theta_d$). In the static contact angle formulation, θ_s is generally chosen to be equal to the equilibrium angle. In the dynamic case, an additional empirical model is used to determine the contact angle dependence on other flow conditions and fluid physical properties (e.g. fluid-fluid surface tension and fluids viscosity) and the surface material properties (friction coefficient, advancing/receding contact angle). It is important to highlight here that the contact angle θ_i is not necessarily the apparent contact angle θ_{app} observed experimentally which varies based on the resolution of the measurements method.

Various contact line models have been derived from either macroscopic models (Hydrodynamic theory) or microscopic models (Molecular Kinetics theory). Some models require that certain parameters be determined from experimental data fitting. A short review of the most commonly used models for calculating the dynamic contact angle is available in Saha and Mitra (2009). In the present study, the model developed by Kistler (1993) is used with the contact angle determined by Eq.11

$$\theta_i = \theta_d = f_H(Ca_{slip} + f_H^{-1}(\theta_e)) \quad (11)$$

$$f_H[x] = \arccos \left\{ 1 - 2 \tanh \left[5.16 \left(\frac{x}{1 + 1.31x^{0.99}} \right)^{0.706} \right] \right\} \quad (12)$$

where $f_H^{-1}(\theta_e)$ is the inverse of the "Hoffman's" empirical function and Ca_{slip} is the capillary number calculated using the interface slip velocity at the solid boundary. This model has previously been coupled with the VOF method (Sikalo et al., 2005; Roisman et al., 2008) or the front tracking method (Muradoglu and Tasoglu, 2010) for the study of the drop impact on partially wetting surface and results were shown to improve the correctness of the simulation of the drop recoil when compared to the static contact angle.

The methods which track implicitly the interface at solid boundaries where a no slip condition is imposed require that a suitable slip law be used to allow contact line motion (Fukai et al., 1993) in spite of the velocity boundary condition. In a Finite Volume VOF method, the non zero velocity at the cell face centers used to advect the volume fraction is implicitly used to move the interface. The slip velocity in this case is mesh dependent and a function of the face center to wall distance. The slip velocity can also be calculated explicitly from a slip length rather than the mesh size using the Navier slip law,

$$u_{slip} = \lambda \dot{\gamma} \quad (13)$$

where λ is the slip length, $\dot{\gamma}$ is the shear rate at the interface, and u_{slip} is the slip velocity at the interface. All results presented in this study are based on the static contact model except for section 4.5 which considers the effect of dynamic model based on Eqs. 11 and 12 with slip velocity taken either as the wall adjacent velocity or the slip velocity as defined by Eq. 13.

3. Problem description

3.1. Numerical domain and grid

The present study considers single gas bubbles rising freely in a quiescent liquid column before impacting and bouncing on a horizontal solid surface. The bubble is initially positioned at a distance $1.5D_{eq}$ from the bottom wall of the numerical domain where D_{eq} is the bubble equivalent diameter. The physical properties of the bulk liquid, gas phase, surface property through the equilibrium contact angle and the bubble characteristics are shown in Table 1. Two different bulk fluids are used in the present work; water and water-glycerol solution (Fluid A). The acceleration in the gravitational direction is $g = 9.81 \text{ m/s}^2$. Different fluid and flow conditions are considered for comparison against experimental data from a range of published and

new studies. The problem is studied using a wedge-like axi-symmetrical domain as sketched in Fig. 1 when appropriate and a 3D model in cases where the bubble trajectory is found to deviate from the vertical direction at any stage of the rise or bounce. The validation cases selected involve Reynolds ($Re = \rho_l D_{eq} V_\infty / \mu_l$), Weber ($\rho_l D_{eq} V_\infty^2 / \sigma$), and Capillary ($Ca = V_\infty \mu_l / \sigma$) numbers in the range (202 – 830.5), (2.13 – 3.69) and (0.004-0.0156), respectively. As confirmed by the bubble shape regime map produced by Bhaga and Weber (1981), the terminal bubble shape before impact is oblate ellipsoidal in all cases. The solid surfaces used are all hydrophilic satisfying equilibrium contact angles measured on the side of liquid phase always lower than 90° .

Figure 1: Schematic diagram of the numerical domain and the boundary conditions for axi-symmetrical simulations.

The width of the numerical domain is defined in terms of the bubble equivalent diameter according to $W = 8D_{eq}$ to avoid any confinement effects (Mukundakrishnan et al., 2007). This criteria is broadly in line with other free rise studies as summarized in Table 2. A height of 30 mm was used in most models. This ensures that the bubble reaches its terminal shape and velocity before collision but also corresponds to the height adopted in the experimental work of Zenit and Legendre (2009) and Kosior et al. (2012). For benchmarking purposes, the height was reduced to 10 mm in the 3D simulations to keep the computational time within a practical limit.

The domain is meshed using orthogonal and uniform cells of constant size Δx . In the axi-symmetrical domain, Δx is the radial width and height of the square cell section. In the 3D domain the cell depth is also uniform and equal

to Δx . Results from a mesh convergence analysis of the bubble terminal velocity and shape (Aspect ratio) are reported in Table 3 for $D_{eq} = 1.48$ mm and the air/water mixture, and Table 4 for $D_{eq} = 2.62$ mm and the air/fluid A mixture. The discretization error between successively refined grids is calculated with reference to the finer mesh. For a quantity ϕ , this discretization error between grids Δx and $\Delta x/2$ is defined by $E_\phi = 100 \times (\phi_{\Delta x} - \phi_{\Delta x/2})/\phi_{\Delta x}$. The mesh size to time step ratio was fixed to $\Delta x/\Delta t = 0.1$. This condition gave bubble terminal characteristics similar to those achieved with an adaptive time step based on a Courant number ($Co=0.25$). In all cases, reductions in the discretization error of 2% or less were achieved by refining the mesh from 25 – 30 to 52 – 59 cells per bubble diameter. A discretization of between 25 to 30 cells per bubble diameter is used thereafter.

3.2. Boundary Conditions and Boundary Mesh Treatment

The boundary conditions are sketched in Fig. 1 using the axi-symmetrical case for illustration. At the lower and side walls, a no slip boundary condition is applied. In few of the test cases, gas is injected into the domain through an injection orifice (not shown) centered on the lower wall. An out-flow boundary is then required and is located over part of the upper wall. It is modeled as a uniform pressure condition. At the upper wall, the contact angle boundary condition is applied. It becomes effective as a portion of the bubble's interface enters the wall adjacent cell and can force the TPCL to form sooner than physically justified. Liquid films of few micrometers thickness can form and persist over significant time intervals as the bubble bounces. In the cases studied here, the film maximum thickness is shown to vary from the order of few tenth of micro meters down to $4 \mu\text{m}$ while lower maximum thicknesses have also been reported ($2.7 \mu\text{m}$ for a 0.14 mm diameter air bubble in water (Krasowska et al., 2003), $\sim 2.5 \mu\text{m}$ for a 0.77 mm diameter air bubble in water (Hendrix et al., 2012)). The implication for mesh requirements is obvious. Therefore, even though an orthogonal and uniform mesh is used everywhere else in the computational domain, the effect of mesh refinement at solid surfaces is also studied. Two different meshes will be considered (i) the Regular mesh made of uniform quadrilateral cells without refinement and (ii) the Refined mesh where the wall adjacent cells are subdivided into 10 cells in the direction perpendicular to the wall with a min/max cell thickness ratio of 0.1 as illustrated in Fig. 2. This produces a wall adjacent cell with minimum thickness $\Delta x_b = 1.2\mu\text{m}$ and an average growth ratio between successive refined cells of 1.29.

Figure 2: A schematic diagram of the mesh subdivision in the Refined case at the upper wall boundary.

3.3. Experimental setup

Part of the numerical validation involves comparison against experimental measurements following a similar procedure to that described by Donoghue et al. (2014). The experimental apparatus used for this purpose consists of a tank of $110 \times 95 \times 195 \text{ mm}^3$ constructed from 3 mm thick glass with a horizontally mounted test surface placed at the top and is illustrated in Fig. 3. The tank contains an adjustable bubble injection orifice. The impact structure sits atop the tank, with the foil being submerged 3 mm below the surface of the water. The impact surface consists of a $10 \text{ }\mu\text{m}$ thick, $70 \times 81.5 \text{ mm}^2$ Constantan[®] foil (Cu55/Ni45) manufactured by Goodfellow. This foil is bonded between two copper bus bars measuring $10 \times 10 \times 84 \text{ mm}^3$, which are used to tension the foil. A metal foil was chosen for its wettability characteristics with water as well as for secondary non-adiabatic studies, which are the focus of a separate study conducted in parallel.

In order to control the size of bubble's generated, two orifice inserts were manufactured from stainless steel, with internal diameters of 0.5 and 1 mm . These inserts screw into the adjustable injection surface, until level with that surface. From the base of the inserts a silicone tube, with an internal diameter of 0.8 mm , connects the orifice to a gas tight syringe. A Hamilton (GASTIGHT 1002 series) 2.5 ml syringe was utilised. The gas flow rate was controlled by a medical grade infusion pump manufactured by *kdScientific* (KDS 200 cz), which allows the selection of the specific model of syringe employed. From tables programmed into the pump, the infusion pump is

capable of supplying the pre-set gas flow rate up to a maximum of 300 *ml/hr*. The total length of tubing used is 400 *mm*. In order to mitigate the effects of a height differential, the infusion pump was placed at the same vertical height as the injection orifice. Once the pump is activated, at a specified injection rate, a stepper motor rotates a threaded bar which moves a ram to compress the plunger of the syringe. Once a single bubble is injected, the pump is stopped. The bubble injection system is mounted on a movable platform, which allows the injection point to be adjusted to varying distances from the test surface. The tank is filled with distilled water which is maintained at a temperature of $22 \pm 0.5^\circ\text{C}$.

Two NAC Hi-Dcam II high speed digital video cameras and pci boards are used to record the bubble motion. The cameras are both controlled by a dedicated computer using the *Lynk-sis* camera software. Both cameras can be synchronized by means of a signal cable from the master camera to the slave pci board; this ensures that both cameras start recording simultaneously. Each camera is capable of frame rates up to a maximum of 20000 *fps*, depending on the resolution. The maximum frame rate at full resolution is 250 *fps*. For these experiments, the cameras recorded at 1000 *fps* with an exposure time of 0.0005 *s*, this corresponds to a resolution of 1280×512 *pixels*. This set-up ensures sharp, crisp images, along with adequate temporal detail. Both cameras are mounted to an aluminium structure, perpendicular to one other. The cameras are fitted with two identical Nikon 50 *mm* f/1.4 AF NIKKOR lenses, attached to 12 *mm* extension tubes. These lenses were chosen as they offer very low image distortion, i.e. image barrelling. Even with the attachment of the extension tubes, which increases magnification, very little distortion was observed; this was verified by means of a reference grid. The lens aperture was set to f/5.6; this ensured sufficient depth of focus for the current set-up.

Illumination of the test area is provided by 3×3 Light Emitting Diode's (LED), per camera. In order to diffuse the light, high quality tracing paper is placed between the LED's and the side face of the tank. The diffusers ensure even light distribution, giving the bubble a dark outline, while providing an almost white background. The LED's are CREE X-Lamp, with each LED having a luminous flux of approximately 260 *lm*, while drawing almost 3 *W* of power each. The color of the LED's is "neutral white", which is best suited for the present study. The LED's were over-driven, to provide an approximate luminous flux of 380 *lm*, with each set consuming 28.8 *W*.

4. Results and discussion

4.1. Free bubble rise

The geometrical properties, terminal shapes, path trajectories, and wakes generated by gas bubbles in free rise in liquids covering a wide range of Morton numbers for both pure and contaminated systems has already been extensively studied experimentally (Bhaga and Weber, 1981; Fan and Tsuchiya, 1990; Saffman, 1956; Clift et al., 1978) and numerically with a range of two fluid flow methods [Front tracking Hua and Lou (2007); Lattice Boltzmann (Amaya-Bower and Lee, 2010); VOF (Annaland et al., 2005); Level Set (Sussman et al., 1998); sharp interface (Ohta and Sussman, 2012)]. Accurate free rise modeling is not the main focus of the present work, but is essential to achieve the correct pre-impact conditions and to allow comparison against benchmark data.

This initial free rise validation focuses on the bubble terminal velocity (V_∞) and aspect ratio (AR). Predictions for bubble rise in a clean water (no surfactant contamination) are compared in Fig. 4 against experimental data from a number of published studies. Furthermore, the bubble terminal aspect ratio is compared against the empirical correlation ($AR = 1/(1 - (9/64)We)$) proposed by Legendre et al. (2012) for water systems with aspect ratios less than three. The present numerical results involve the two bulk liquids (water and fluid A) and the four bubble diameters ranging from 1 mm to 2.62 mm listed in Table 1. The experimental data of Fugasova-Zednikova et al. (2010) shows a scattering around the curve produced by Moore's correlation. This was attributed by the author to differences in the bulk liquid temperature between experiments. The experimental data of Duineveld (1995) compares well with the Moore curve at small bubble equivalent diameters. However, a small difference is noticed for larger equivalent diameters. The numerical results compare well with Moore's correlation (Moore, 1965) and are within a reasonable uncertainty range of other experimental data (particularly given the relatively large variability between data at similar flow conditions).

Errors in the bubble terminal velocity ($E_{V_\infty} = 100 * [(V_{exp} - V_{num})/V_{exp}]$) and aspect ratio ($E_{AR} = 100 * [(AR_{exp} - AR_{num})/AR_{exp}]$) are calculated with respect to selected experimental data and shown in Table 5. For a bubble diameter of 1.48 mm, the numerical simulations provide bubble terminal velocities with relative errors of 6.94% and 2.72% compared to results provided by Kosior et al. (2012) and the Moore correlation. Similar error levels are found for bubble diameter 2.62 mm and the air/fluid A mixture. The

Figure 3: Schematic representation of experimental setup.

Figure 4: A comparison of the bubble terminal velocity from different experimental, empirical, and numerical data.

terminal velocity obtained experimentally by Duineveld (1995) is noticed to be larger than those predicted numerically and obtained by the Moore correlation with approximate errors 8% and 3% respectively. The numerical simulations appear to over-predict the terminal velocity for bubble diameter 1.58 mm by comparison to data from Tsao and Koch (1997). In this case, however, the influence of impurities in the liquid used in the experiments can explain the lower bubble terminal velocity. The accumulation of contaminants at the bubble surface can reduce the interface mobility and increase drag (Malysa et al., 2005). The numerical predictions of the bubble aspect ratio are shown to produce larger relative errors ranging from 15% to 7.8% when compared with experimental data although this is reduced to $E_{AR_{emp}} = 2\%$ when compared with the empirical values AR_{emp} calculated from the correlation proposed by Legendre et al. (2012) with $E_{AR_{emp}}$ is calculated as $(E_{AR_{emp}} = 100 * [(AR - AR_{emp})/AR])$.

For $D_{eq} = 1.48$ mm and air/water mixture, the bubble has also been tested in 3D primarily to test the validity of the axi-symmetrical assumption. Results produced relative differences in the bubble terminal velocity and aspect ratio equal to 0.1% and 2%, respectively. The model also confirmed the predominantly rectilinear characteristic of the rise trajectory (with a deviation from the centerline lower than 0.02 mm). For the air/fluid A mixture and $D_{eq} = 2.62$ mm, similar conclusions were obtained by Zenit and Legendre (2009).

4.2. Mechanism of bubble bouncing

A brief description of the bubble impact and bounce is given here before assessing the solution accuracy. A sequence of the bubble interface defined as the iso-contour plot of $\alpha = 0.5$ is given in Fig. 5 to illustrate a typical interaction sequence between the bubble and the solid surface during the first bounce cycle. These results were obtained with a Refined mesh for the air/water mixture with $D_{eq} = 1.48$ mm. At the initial stage (Frames 1-3), the bubble approaches the wall with its terminal velocity and shape and is still unaffected by the upper boundary. At a distance $1.5D_{eq}$ (Frame 4), the bubble begins to decelerate before flattening rapidly under the combined effect of buoyancy and increasing forward pressure (Frame 5-6). As the bubble continues to approach the wall (Frame 7-8), a thin liquid film forms between the bubble and the wall. The bubble velocity continues to decrease rapidly down to zero at which point the bubble has reached its maximum deformation. The bubble kinetic energy has then been transferred to surface deformation

energy. Under current conditions, no direct contact forms between the air inside the bubble and the solid surface so that the liquid film does not break and no triple contact line exists. The restitution process begins when the bubble starts to rebound creating a cusped tail shape (Frame 9). This tail forms as the liquid film expands and eventually disappears as the bubble moves away from the wall (Frame 10-13). The filling in of the liquid film increases rapidly generating pressure fluctuations which manifests themselves as large oscillations in the bubble interface. The bubble recovers its spherical shape as its velocity decreases back to zero once again (Frame 14-17). At this stage, the bubble resumes its upward motion starting the second bouncing cycle. The number of rebounds varies with the fluid and flow properties but also the solid surface properties which will dictate whether a TPCL forms or whether a liquid film stabilizes. Qualitatively similar behaviors have been observed experimentally with air/water mixtures (Tsao and Koch, 1997) and heavier liquids (Legendre et al., 2005; Zenit and Legendre, 2009).

4.3. Numerical Model Validation

The main purpose of this validation is to determine the importance of correctly resolving the liquid film and modeling its influence on the bubble dynamics. Two main test cases are considered to account for the effect of hydrophilic surfaces of varying strength. Flow conditions in these cases justify the use of an axi-symmetrical model and one additional test is included to consider full 3D conditions.

4.3.1. Influence of Mesh Refinement

The influence of the mesh resolution in the region immediately adjacent to the upper wall is assessed against experimental data from Zenit and Legendre (2009) and Kosior et al. (2012). The two cases are characterized by:

- Case I; (Zenit and Legendre, 2009): Mixture of air and Fluid A with a bubble of diameter $D_{eq} = 2.62$ mm and an equilibrium contact angle $\theta_e = 30^\circ$.
- Case II; (Kosior et al., 2012): Mixture of air and water with a bubble of diameter $D_{eq} = 1.48$ mm and an equilibrium contact angle $\theta_e = 0^\circ$.

Although the two test cases relate to different fluid properties and bubble diameters, the parameter of primary interest in the present analysis is the equilibrium contact angle. It is important to note that this is not intended as

Figure 5: Bubble interface shown as iso-contour of $\alpha = 0.5$ during the first bouncing cycle. The sequence starts at top left (Frame 1) and progress to the bottom right (Frame 25) at intervals of 0.002 s. The computations were for the air/water mixture with $D_{eq} = 1.48\text{mm}$ and the Refined mesh.

comparative study but as an assessment of the impact of the mesh resolution under fundamentally different surface conditions. With a surface equilibrium contact angle $\theta_e = 0^\circ$ the surface is highly hydrophilic and a liquid layer is in contact with the surface at all stages of the bounce cycle. With $\theta_e = 30^\circ$ the TPCL is known to form under certain conditions. This initial analysis considers both the Refined and Regular meshes using the static contact angle boundary condition.

For Case I, results are presented in terms of the bubble center of gravity (CGy), velocity (V_b), and aspect ratio (AR) as shown in Figs. 6, 7 and 8 and only include the first bounce cycle for consistency with the benchmark data. Both meshes provide numerical results which are similar to the experimental data up to the impact and slightly beyond. The amplitude of rebound however is larger with the Refined mesh and closer to the experimental values. With the Regular mesh the liquid film is found to drain entirely much sooner than with the Refined mesh. The formation of the TPCL can have a non negligible effect on the dynamics of the bubble. As the film breaks, the bubble can appear to stick to the surface. Although this is physically consistent with a hydrophilic surface, the contact angle boundary condition can artificially increase the effect. The boundary condition is imposed as soon as the interface enters the wall adjacent cells even if its size is much larger than the active range of Van der Waals forces. A coarse mesh can therefore be expected to induce an earlier TPCL formation and to effectively attract the bubble towards the surface. The bubble velocity and aspect ratio show lower sensitivity to the mesh although some improvements in prediction with the Refined case are still noticeable.

With Case II, the liquid film should stabilize precluding any TPCL formation. The bubble velocity is shown in Fig. 9 over several bounce cycles in this case. The time ($t = 0$) is the moment when the bubble is at its maximum deformation close to the wall. This corresponds to the time when the bubble velocity changes its sign. Both mesh cases give results that are in broad agreement with the experimental data, but small although non negligible differences in the maximum velocity during the first bouncing cycle are also shown. The difference however is consistent with the difference in the bubble terminal velocity before impact against the wall. Both the bubble velocity plots and contour visualizations (not shown here) confirm that the bubble eventually stops bouncing. Results also confirm that a thin liquid film is always present with the Refined mesh but not with the Regular mesh. The TPCL formation is shown to have an effect on the velocity but the small

Figure 6: Bubble center of gravity for Case I: $D_{eq} = 2.62$ mm and the air/Fluid A mixture. Computational results with Refined and Regular mesh. Experimental results from Zenit and Legendre (2009)

Figure 7: Bubble Vertical velocity for Case I: $D_{eq} = 2.62$ mm and the air/Fluid A mixture. Computational results with Refined and Regular mesh. Experimental results from Zenit and Legendre (2009)

Figure 8: Bubble aspect ratio for Case I: $D_{eq} = 2.62$ mm and the air/Fluid A mixture. Computational results with Refined and Regular mesh. Experimental results from Zenit and Legendre (2009)

changes involved make it difficult to draw definite conclusions in this case. Similar arguments can be made with respect to the bubble aspect ratio plots shown in Fig. 10. These show the same small and rapid oscillations as observed experimentally following the first rebound as the bubble returns to its initial spherical shape. The three main troughs and peaks corresponding to bubble flattening at impact and bubble stretching during rebound are predicted by both meshes with similar magnitude. In this case however, the peaks from the Refined mesh appear to be more notably in phase with experimental data.

Two main conclusions can be drawn from the study of the two cases above. Firstly, the contact angle formulation is likely to have a limited impact on the results once the liquid film is correctly resolved. Secondly, a coarse mesh is likely to induce significant errors with larger contact angles which tend to promote early TPCL formation and dampen quickly the bouncing process. More generally, correctly capturing the liquid film is essential for accurate prediction of the bubble bounce in particular when dealing with hydrophobic surfaces.

4.3.2. Bouncing dynamics in 3D flow

The 3D test case involves a single isolated air bubble in water generated from a wall orifice at the bottom surface of the domain and modeled with the

Figure 9: Bubble velocity for Case II: $D_{eq} = 1.48$ mm and the air/water mixture. Computational results with Refined and Regular mesh. Experimental results from Kosior et al. (2012)

Figure 10: Bubble aspect ratio for Case II: $D_{eq} = 1.48$ mm and the air/water mixture. Computational results with Refined and Regular mesh. Experimental results from Kosior et al. (2012)

533 "Refined" mesh. The same bubble growth, detachment and rise conditions
534 as those in previous publications (Albadawi et al., 2012, 2013) are considered
535 here. Two bubble diameters $D_{eq} = 2.62, 3.3$ mm corresponding to wall orifices
536 diameters 0.5, 1 mm are included. Based on Clift et al. (1978) and Fan and
537 Tsuchiya (1990), both bubbles should assume a slightly zig-zaging trajectory
538 shortly after detachment, but the domain height is kept relatively small at
539 10 mm to limit the 3D effect. The bubble at this height does not reach its
540 terminal velocity. The advancing contact angles on the upper surface was
541 measured experimentally to be 24° . This was achieved by studying the profile
542 of an equilibrium droplet on the Constantan surface. The measured angle
543 of 24° is used in the numerical model to determine the static contact angle
544 with Eq. 10.

545 The numerical prediction of the 3.3 mm bubble trajectory is plotted in
546 Fig. 11. Although the bubble rise is predominantly rectilinear, it does move
547 freely in all directions after impact and, after the first two bounces, oscillates
548 consistently towards the right hand side boundary. This motion is believed
549 to be influenced by the wake generated behind the bubble during its rise
550 (Donoghue et al., 2012). A sequence of snapshots of the bubble interface
551 viewed from a vertical plane is given in Fig. 12 for the first bounce cycle.
552 Before reaching the upper surface, the bubble is shown to have an ellipsoidal
553 shape with a plane symmetry (at $t = -0.006$ s). After that point, it deforms
554 rapidly due to the collision with maximum deformation at the time ($t = 0$
555 s). When the bubble rebounds, it takes a seemingly random shape.

556 The bubble center of gravity and velocity are compared against experi-
557 mental data in Fig. 14 and Fig. 15, respectively. The time $t = -0.05$ s in
558 Fig. 15 corresponds to the moment when the bubble starts pinching off the
559 injection orifice. After detachment, the bubble rises freely and its velocity
560 increases quickly. The numerical predictions in Fig. 14 are shown to be gen-
561 erally very close to the measured data for the full process apart from the
562 first rebound which shows a significant overshoot in the maximum rebound
563 distance with an error of 25% compared to the experiments (See Table 6).
564 This discrepancy could be attributed to differences in the amplitude and
565 frequency of interface oscillations. Comparing numerical and experimental
566 side views of the bubble over the first bounce cycle (Figs. 12 and 13) con-
567 firms some notable differences. The experimental bubble shape is shown to
568 preserve symmetry after the first bounce while the numerical predictions in-
569 dicate significant shape distortions. This is most likely due to numerically
570 induced spurious currents but interestingly it is also shown not to impact on

Figure 11: Trajectory of the air bubble in water predicted numerically with $D_{eq} = 3.3$ mm.

Figure 12: Sequence of screen shots for the numerical predictions modeled using the Refined mesh of colliding 3.3 mm air bubble in water . The contour plots are given from $t = -0.024$ s (top left) to $t = 0.042$ s (bottom right) at time intervals of 0.006 s between each two successive frames.

Figure 13: Sequence of screen shots for the experimental observations of colliding 3.3 mm air bubble in water . The contour plots are given from $t = -0.024$ s (top left) to $t = 0.042$ s (bottom right) at time intervals of 0.006 s between each two successive frames.

the accuracy of the mean trajectory of the bubble center of gravity or on its velocity over the successive rebounds (Figs. 14 and 15). The sequence of shape visualizations fails however to highlight higher frequency oscillations in the bubble aspect ratio. These oscillations have been measured experimentally and have been found to persist from the time of release from the injection hole. In the case of the results reported here, the oscillations are shown to preserve symmetry. The aspect ratio measured experimentally oscillates between 1.17 and 1.05 with a period of about 4 ms. The numerical predictions do not reproduce this which could explain the difference in the amplitude of the first rebound. It is indeed possible but difficult to verify that lower surface deformation energy translates in lower rebound amplitude. Interestingly it is seen that the experimental bubble velocity data (Fig. 15) shows rapid oscillations about a mean value which is close to the numerical predictions. This is consistent with rapid surface oscillations due to bubble shape oscillations. Depending on the deformation stage just before impact, one can conceive a larger or smaller rebound amplitude about its mean. Other observations which would tend to confirm these suggestions is the fact that in the case of the smaller $D_{eq} = 2.62$ mm bubble the rebound amplitude is under predicted rather than over predicted (see Fig. 14). The errors in the bubble maximum rebound distance compared to the experimental data for the first six bouncing cycles are summarized in Table 6. Two errors are given for the bubble center of gravity, one is calculated numerically using the projected area of the bubble (2D) and the other using the bubble total volume (3D). This table confirms that the numerical results provide a good quantitative comparison for the full bouncing process with errors lower than 8 % in all cases apart from the first rebound.

4.4. *Film formation and drainage*

Accurate modeling of the liquid film formation and drainage is clearly important. Focus is turned here to this aspect of the process. A time sequence of the 3D contour of the 3.3 mm diameter air bubble after impact and viewed from the upper surface of the domain is shown in Fig. 16 to illustrate the extent of the film in the horizontal plane. Of particular interest is the clear formation of a dimple centered on the approximate axis of symmetry of the bubble. The liquid film trapped between the approaching bubble and the wall is initially uniformly distributed but as it drains under the action of buoyancy, the bubble spreads outward and the film thickness is shown to reduce more rapidly toward its outer rim creating the observed dimple in the

Figure 14: Comparison of bubble center of gravity with experimental data with the air/water mixture and equivalent diameters (a) $D_{eq} = 3.3$ mm and (b) $D_{eq} = 2.62$ mm using a Refined mesh.

Figure 15: Comparison of bubble velocity in the gravitational direction with experimental data with air/water mixture and $D_{eq} = 3.3$ mm and Refined mesh.

608 bubble surface. This dimple is at its largest at the first bounce and reduces
 609 rapidly over successive bounces along with the spreading, in the horizontal
 610 plane, of the film and interface outer rim. As the kinetic energy of the bubble
 611 dissipates after successive rebounds, a stage is reached where, the liquid film
 612 either drains to a minimum thickness and stabilizes or a TPCL forms. The
 613 steady state is determined by the surface properties, i.e. on the contact angle
 614 boundary condition.

Figure 16: Sequence of screenshots illustrating the size of the maximum film formed at each bouncing cycle on the bubble top surface during collision, with air/water mixture and $D_{eq} = 3.3$ mm and Refined mesh.

615 An axi-symmetrical model of a $D_{eq} = 1.48$ mm air bubble in water is
 616 considered next to provide a more detailed description of the film and dimple
 617 evolutions over time. Two static contact angles $\theta_{app} = 0^\circ$ and $\theta_{app} = 30^\circ$
 618 are included and the Refined mesh is used to ensure that the liquid film
 619 is adequately captured at least over the first rebounds. The plots of the
 620 bubble interface at successive times over the advancing phase of the first
 621 bounce are given in Fig. 17 at 0.2 ms time intervals. As no TPCL forms
 622 at this stage, the static contact angle does not influence the process. The
 623 dimple formation starts when the bubble wall separation distance reaches
 624 approximately $\sim 50\mu\text{m}$ which is twice the value proposed by Klaseboer et al.

(2000) ($\sim 0.4R_{eq}\sqrt{2Ca} = 28 \mu\text{m}$). The minimum height of the dimple at the axis of symmetry is approximately $35 \mu\text{m}$ while the film thickness reduces to a much smaller $\sim 15 \mu\text{m}$ toward the rim of the bubble. The plot also confirms the radial spreading of this outer rim from the axis of symmetry.

Figure 17: Film formation during the first bubble approach to the wall with contact angle 0° for air/water mixture and $D_{eq} = 1.48 \text{ mm}$.

The static contact angle has a significant influence on the last stage of the process as it reaches steady state. When the contact angle is set to 0 in the numerical model, a continuous film stabilizes between the bubble and the solid wall (Fig. 18a). Physically, this occurs when in contact with a hydrophilic surfaces as observed by Kosior et al. (2012). The film outer radius in the horizontal plan tends to $180 \mu\text{m}$ as it stabilizes; a value which is close to that suggested by Kosior et al. (2012) ($\sqrt{2R_{eq}^4\Delta\rho g/3\sigma} \approx 168 \mu\text{m}$). When the equilibrium contact angle is greater than zero, a TPCL forms expanding outward until the imposed static contact angle is satisfied ($\theta_{app} = 30^\circ$ in Fig. 18b).

The minimum film thickness at successive rebounds for both the $D_{eq} = 1.48 \text{ mm}$ air bubble in water system (case II) and the $D_{eq} = 2.62 \text{ mm}$ air bubble in FluidA (case I) are given in Table 7. This is presented along with the bubble kinetic energy ($KE = 0.5C_M\rho_l V_B V^2$) and potential energy ($PE = \Delta A\sigma$), where ΔA and V are the changes in the bubble area, and the maximum rise velocity during the collision process at each rebound, respectively, V_B is the bubble equivalent volume, and $C_M = 0.62AR - 0.12$

(a) Contact angle 0°

(b) Contact angle 30°

Figure 18: Film formation during the last bounce with the air/water mixture, $D_{eq} = 1.48$ mm and contact angles (a) 0° and (b) 30° . The arrow is in the direction of time increase and successive plots are at time intervals of 0.4ms

is the added mass coefficient (Klaseboer et al., 2001). Not surprisingly the minimum film thickness is shown to decrease after each bouncing cycle until the film ruptures and the TPCL forms. Similar observations were made by Doublier (1991) in the case of collision with a free surface. The minimum thickness found here for case II was $4.8 \mu\text{m}$ which is four times the mesh size across the film. This value is of the same order as those observed and predicted experimentally in Tsao and Koch (1997) ($O(10\mu\text{m})$), (Hendrix et al., 2012) ($2.5 \mu\text{m}$) for $D_{eq} \sim 0.7 \text{ mm}$, and in (Krasowska et al., 2003) ($2.7 \mu\text{m}$).

Also for both cases presented in Table. 7, the bubble fails to rebound when its kinetic energy falls below $KE \sim 3 \times 10^{-9} \text{ J}$. A similar threshold value was found experimentally by Zawala et al. (2007) with a $D_{eq} = 1.47 \text{ mm}$ air bubble in water. The author reported a similar behavior with several rebounds ending when the bubble kinetic energy fell below $10 \times 10^{-9} \text{ J}$ whereas bouncing was shown to occur when this value was above $1 \times 10^{-7} \text{ J}$. Another interesting observation is the relationship between the film thickness and radius. The larger kinetic energy is found to generate larger projected contact areas between the bubble and the wall so that a larger film is generated requiring longer periods of time to drain. This, in turn, leads to a longer bouncing cycle period.

Tsao and Koch (1997) have argued from experimental observation that the formation of a surface dimple and the drainage of the liquid film were consistent with a peak in liquid pressure above the rising bubble prior to impact. This existence of a high pressure region however could not be reproduced by the numerical model of Sanada et al. (2005). The modified pressure (P_{rgh}) along a horizontal line parallel to the upper wall at a distance of $5 \mu\text{m}$ is plotted in Fig. 19. These results correspond to the $D_{eq} = 1.48 \text{ mm}$ air bubble in water case solved with the Refined mesh during the first bounce. The pressure profile is shown at several time steps starting from ($t_a, Approach$) when the bubble upper interface is at a distance 0.52 mm from the wall and ending at time ($t_f, Recede$) at a distance 0.02 mm following impact. The pressure is shown to increase by a factor of four over a short period of time (5 ms).

A comparison of pressure contours and velocity plots provides some useful insight. Fig. 20 combines both data prior to and following impact and rebound when the bubble is approximately at 0.5 mm from the wall. The intensity of the velocity field in the liquid region is depicted using an off-scale vector plot with color variation from red (large value) to blue (small value). A similar color grading is used for plotting the pressure variation using 10

Figure 19: Horizontal pressure distribution at $5 \mu\text{m}$ from the wall during the first bouncing cycle with air/water mixture, $D_{eq} = 1.48 \text{ mm}$.

iso-contour lines dividing the full changes in the pressure. The black solid line in the figure represents the bubble interface with iso-line ($\alpha = 0.5$). As the bubble approaches the wall prior to impact, the liquid flows radially outward in the film region and from high pressure to low pressure regions. After the rebound, the liquid flows in the opposite direction and against adverse pressure gradients leading to some localized flow reversal and separation near the axis of symmetry. This along with the the acoustic radiation of energy resulting from the bubble shape oscillations during the rebound have been suggested as the main source of energy dissipation by Tsao and Koch (1997).

4.5. Dynamic contact angle model

Once the film ruptures and the TPCL forms, the influence of the surface properties in the form of surface tension becomes significant. This is interpreted numerically by the contact angle boundary condition. The sensitivity of computational results to boundary conditions is assessed here by reference to the bubble velocity considering three contact angle formulations (static, dynamic with and without slip velocity model) and the two mesh types (Refined and Coarse). This section focuses on the case of a $D_{eq} = 1.48 \text{ mm}$ diameter bubble in water with a surface contact angle of 30° . The Coarse mesh model is used to assess the sensitivity of the contact formulation with

Figure 20: Velocity vector plot at two different stages of bouncing. The scale of the velocity vector is set to off. The color range is from red (large) to blue (small), (a-left) approach stage with velocity magnitude range $[0, 0.259 \text{ m/s}]$ and pressure range $[-100, 63 \text{ kg/m.s}^2]$, (b-right) recede stage with velocity range $[0, 0.191 \text{ m/s}]$ and pressure range $[-100, 206 \text{ kg/m.s}^2]$, with angle 0° and air/water mixture, $D_{eq} = 1.48 \text{ mm}$.

an unsuitable mesh as the TPCL forms directly at the first bouncing cycle. With the dynamic no slip model, the bubble slip velocity at the wall boundary is calculated as the tangential velocity of the neighboring cell center so that results can be expected to be influenced by the mesh resolution near the wall. In the case of dynamic slip model, the slip velocity is calculated in terms of the velocity gradient in the vertical direction to the wall (Eq. 13) with $\lambda = 0.1\Delta x$. The value of λ is chosen so that it is of the order $O(10)$ μm and $O(0.1)$ μm with the Regular and Refined mesh, respectively. As shown in Fig. 21, the impact of the contact model is, as expected, most noticeable with the Coarse mesh due to the early formation of the TPCL. Fig. 21b clearly shows that the no slip model induces large and unphysical velocity fluctuations which are found to correlate with bubble shape oscillations. Both dampen slowly with time. The slip model compares well with the static contact angle model and matches the experimental results reasonably well. When the mesh is refined to capture the liquid film (Fig. 21a), the results show very little sensitivity to the contact angle formulation. The comparison between the two meshes show that capturing the TPCL with an adequate mesh resolution reduces the influence of the contact angle model and that the static contact angle model is sufficient. It is worth noting as well that some oscillations persist with all models, a behavior which is not observed experimentally and can be explained by spurious currents. Most interesting is the fact that very similar results are observed with the case of $D_{eq} = 2.62$ mm with air/fluid A mixture and equilibrium contact angle 30° (results not presented here). In this case the TPCL forms but this occurs late in the process when most of the kinetic energy has been dissipated due to increased influence of the liquid viscosity. At that stage, changes induced by the contact model have little impact on the bubble velocity.

When the TPCL is formed at the solid surface, the air inside the bubble comes in direct contact with the wall and the three phases (Solid/ Liquid/ Gas) meet at the contact region. A new geometrical parameter, called the spreading radius, can be introduced at this stage. It is the equivalent radius of the non-wetted region at the interface between the bubble and the solid surface. Its time evolution is shown in Fig. 22 for both static and dynamic (with slip) contact angle models considering a $D_{eq} = 1.48$ mm air bubble in water system and an equilibrium contact angle set at 30° to allow TPCL formation. The initial time is set here as the instant when the TPCL forms. Both models show a rapid increase in the bubble spreading radius immediately after the TPCL forms. This is followed by a slow variations of the

Figure 21: Comparison of slip model influence on the bubble velocity during the bouncing process with dynamic contact angle boundary, with $D_{eq} = 1.48$ mm and the air/water mixture, Experiments from Kosior et al. (2012).

radius around an average value (0.4 mm) and both contact model provide globally similar results. A difference appears and grows after 0.025s but remains reasonably small ($O(10) \mu\text{m}$) and is difficult to explain. The bubble instantaneous apparent contact angle is also plotted in Fig. 23 and shows similar trends with a initial rapid increase from (5°) to approximately (25°) before leveling off with larger fluctuations about a globally steady mean. Here again consistent differences between the two models are difficult to identify and justify. In practice both models predict bubble oscillations with a small amplitudes which are of the order ($50 \mu\text{m}$) for the bubble height.

This confirms that similar results can be obtained using either the static or dynamic contact angle model provided that the mesh is sufficiently refined to resolve the liquid film. This can be explained by the small influence of the slip capillary number at the last stages of bouncing [$Ca_{slip} \approx 10 \times 10^{-4}, 4 \times 10^{-4}$] when compared to the case of drop spreading (Sikalo et al., 2005; Yokoi et al., 2009). This in turn reduces the influences of the dynamic model on the apparent contact angle and reduces variations around its equilibrium value ($\theta_d = \theta_e + f(Ca_{slip}) \approx \theta_e$). It is important to mention that for non-regular surfaces where the advancing contact angle is significantly different from its receding and equilibrium values, there may be some justification for using

Figure 22: Evolution of the bubble spreading radius after the TPCL formation for $D_{eq} = 1.48$ mm and air/water mixture with Refined mesh and equilibrium contact angle 30° . The dynamic contact angle model is coupled with a slip boundary conditions.

Figure 23: Evolution of the bubble apparent contact angle after the TPCL formation for $D_{eq} = 1.48$ mm and air/water mixture with Refined mesh and equilibrium contact angle 30° . The dynamic contact angle model is coupled with a slip boundary conditions.

the dynamic contact angle model. However, the influence of contact angle hysteresis can be expected to be more important in cases where bubbles slide and bounce along slightly inclined surfaces where a TPCL may still form and differences in the apparent contact angle may have a stronger influence on the bubble dynamics.

5. Conclusion

A Volume of Fluid model of free bubble rise and impact on and bounce from a horizontal solid surface has been studied. The model's accuracy has been assessed against experiments and existing published benchmark data. It has been shown that:

- The model can predict bubble terminal velocities within 5 % of benchmark experimental data. The computed bubble aspect ratio tends to be larger than the experimental values but provides good comparison with the empirical correlation of Legendre et al. (2012).
- The analysis of the bubble bounce with different mesh resolutions has highlighted the importance of relying on a Refined mesh in the vicinity of solid surfaces. A resolution of the liquid film with 4 cells was found to allow accurate representation of the unsteady process. For coarser mesh sizes, the contact angle boundary conditions force early formation of a TPCL with changes in the amplitude of rebound. The influence of the mesh resolution is dependent on the film thickness and increases with the equilibrium contact angle.
- 3D models capable of dealing with non linear rise and bounce trajectories have confirmed that similar levels of accuracy could be achieved in such cases. Some differences at the first rebound suggest that increased mesh resolution may be required to capture bubble shape oscillations that have been assumed to impact on the amplitude of rebound.
- The numerical model can provide physically consistent descriptions provided that adequate mesh resolution was used. The onset of the dimple formation and the size of the liquid film during the bubble approach were shown to compare well with published empirical correlations or observations. For zero equilibrium contact angle, a continuous

film is always observed beneath the bubble, while for larger contact angles the film ruptures as a TPCL forms. The film thickness decreases after each bouncing cycle along with bubble kinetic energy and the film was found to rupture when the bubble kinetic energy falls below a threshold of $KE = 3 \times 10^{-9}$ J.

- Computations confirmed the presence of a rapidly increasing pressure peak in liquid film prior to impact. The formation of the dimple has been attributed to this increase in pressure. The pressure distribution in the liquid film following impact and during the rebound forces liquid to flow against an adverse pressure gradients. The resulting flow separation previously discussed in Tsao and Koch (1997) was captured by the model.
- A dynamic contact angle model with an implicit slip velocity calculation produced large unphysical mesh dependent oscillations. In contrast both the Navier Slip dynamic and static contact angle models provide bubble velocity predictions shown to be in close agreement with experimental data. The slip Capillary number required for the dynamic contact angle calculation is sufficiently small to explain the limited influence of the dynamic formulation.

Acknowledgements

The authors wish to acknowledge the support of Science Foundation Ireland under its Research Frontiers Programme (grant number 09/ RFP/ ENM2151).

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1002 **Figures Captions**

1003 **Figure 1:** Schematic diagram of the numerical domain and the boundary
1004 conditions for axi-symmetrical simulations.

1005 **Figure 2:** A schematic diagram of the mesh subdivision in the Refined
1006 case at the upper wall boundary.

1007 **Figure 3:** Schematic representation of experimental setup.

1008 **Figure 4:** A comparison of the bubble terminal velocity from different
1009 experimental, empirical, and numerical data.

Figure 5: Bubble interface shown as iso-contour of $\alpha = 0.5$ during the first bouncing cycle. The sequence starts at top left (Frame 1) and progresses to the bottom right (Frame 25) at intervals of 0.002 s. The computations were for the air/water mixture with $D_{eq} = 1.48$ mm and the Refined mesh.

Figure 6: Bubble center of gravity for Case I: $D_{eq} = 2.62$ mm and the air/Fluid A mixture. Computational results with Refined and Regular mesh. Experimental results from Zenit and Legendre (2009).

Figure 7: Bubble Vertical velocity for Case I: $D_{eq} = 2.62$ mm and the air/Fluid A mixture. Computational results with Refined and Regular mesh. Experimental results from Zenit and Legendre (2009).

Figure 8: Bubble aspect ratio for Case I: $D_{eq} = 2.62$ mm and the air/Fluid A mixture. Computational results with Refined and Regular mesh. Experimental results from Zenit and Legendre (2009).

Figure 9: Bubble velocity for Case II: $D_{eq} = 1.48$ mm and the air/water mixture. Computational results with Refined and Regular mesh. Experimental results from Kosior et al. (2012).

Figure 10: Bubble aspect ratio for Case II: $D_{eq} = 1.48$ mm and the air/water mixture. Computational results with Refined and Regular mesh. Experimental results from Kosior et al. (2012).

Figure 11: Trajectory of the air bubble in water predicted numerically with $D_{eq} = 3.3$ mm.

Figure 12: Sequence of screen shots for the numerical predictions modeled using the Refined mesh of colliding 3.3 mm air bubble in water. The contour plots are given from $t = -0.024$ s (top left) to $t = 0.042$ s (bottom right) at time intervals of 0.006 s between each two successive frames.

Figure 13: Sequence of screen shots for the experimental observations of colliding 3.3 mm air bubble in water. The contour plots are given from $t = -0.024$ s (top left) to $t = 0.042$ s (bottom right) at time intervals of 0.006 s between each two successive frames.

Figure 14: Comparison of bubble center of gravity with experimental data with the air/water mixture and equivalent diameters (a) $D_{eq} = 3.3$ mm and (b) $D_{eq} = 2.62$ mm using a Refined mesh.

Figure 15: Comparison of bubble velocity in the gravitational direction with experimental data with air/water mixture and $D_{eq} = 3.3$ mm and Refined mesh.

Figure 16: Sequence of screenshots illustrating the size of the maximum film formed at each bouncing cycle on the bubble top surface during collision, with air/water mixture and $D_{eq} = 3.3$ mm and Refined mesh.

Figure 17: Film formation during the first bubble approach to the wall with contact angle 0° for air/water mixture and $D_{eq} = 1.48$ mm.

Figure 18: Film formation during the last bounce with the air/water mixture, $D_{eq} = 1.48$ mm and contact angles (a) 0° and (b) 30° . The arrow is in the direction of time increase and successive plots are at time intervals of 0.4ms.

Figure 19: Horizontal pressure distribution at $5 \mu\text{m}$ from the wall during the first bouncing cycle with air/water mixture, $D_{eq} = 1.48$ mm.

Figure 20: Velocity vector plot at two different stages of bouncing. The scale of the velocity vector is set to off. The color range is from red (large) to blue (small), (a-left) approach stage with velocity magnitude range $[0, 0.259 \text{ m/s}]$ and pressure range $[-100, 63 \text{ kg/m.s}^2]$, (b-right) recede stage with velocity range $[0, 0.191 \text{ m/s}]$ and pressure range $[-100, 206 \text{ kg/m.s}^2]$, with angle 0° and air/water mixture, $D_{eq} = 1.48$ mm.

Figure 21: Comparison of slip model influence on the bubble velocity during the bouncing process with dynamic contact angle boundary for (a) Refined mesh and (b) Regular mesh, with $D_{eq} = 1.48$ mm and the air/water mixture, Experiments from Kosior et al. (2012).

Figure 22: Evolution of the bubble spreading radius after the TPCL formation for $D_{eq} = 1.48$ mm and air/water mixture with Refined mesh and equilibrium contact angle 30° . The dynamic contact angle model is coupled with a slip boundary conditions.

Figure 23: Evolution of the bubble apparent contact angle after the TPCL formation for $D_{eq} = 1.48$ mm and air/water mixture with Refined mesh and equilibrium contact angle 30° . The dynamic contact angle model is coupled with a slip boundary conditions.

Parameter	Unit	Air	Water	Fluid A
Density	kg/m^3	1.225	998.2	1087
Viscosity	kg/m.s	1.79×10^{-5}	0.001	0.0038
Surface tension	N/m	-	0.072	0.0697
Equivalent diameter	mm	-	1.48, 2.6, 3.3	2.62
contact angle	$^\circ$	-	0, 24	30
Morton number ($g\mu_l^4/\rho_l\sigma^3$)	-	-	2.63×10^{-11}	5.56×10^{-9}
Bond number ($\rho_l g D_{eq}^2/\sigma$)	-	-	0.298-1.48	1.05

Table 1: Fluid physical properties and surface and bubble characteristics.

Authors	Numerical Method	Rig width to bubble diameter ratio
Mukundakrishnan et al. (2007)	Front Tracking Method	8
Bonometti and Magnaudet (2007)	Volume of Fluid	5
Ansari and Nimvari (2011)	Level Set	3-4
Kumar and Delauré (2012)	Volume of Fluid	8
Ohta and Sussman (2012)	Sharp interface method	5
Chakraborty et al. (2013)	Coupled CLSVOF	8
Shu and Yang (2013)	Lattice Boltzmann	5

Table 2: Review of numerical domain width from recent free bubble rise studies.

Δx [mm]	nb of cells/diameter	V_{∞} [mm/s]	AR [-]	$E_{v_{\infty}}$ [%]	E_{AR} [%]
0.2	7.4	156.40	1.242	-	-
0.1	14.8	299.06	1.344	47.702	7.589
0.05	29.6	322.03	1.400	7.132	4.000
0.025	59.2	315.82	1.390	-1.965	-0.719

Table 3: Mesh convergence analysis of bubble in free rise with equivalent diameter $D_{eq} = 1.48$ mm and air/water mixture.

Δx [mm]	nb of cells/diameter	V_{∞} [mm/s]	AR [-]	$E_{v_{\infty}}$ [%]	E_{AR} [%]
0.2	13.1	247.6	1.507	-	-
0.1	26.2	271.4	1.657	8.77	9.052
0.05	52.4	271.6	1.691	0.07	2.010

Table 4: Mesh convergence analysis of bubble in free rise with $D_{eq} = 2.62$ mm and air/fluid A.

Bubble diameter [mm]	Method	V_{∞} [mm/s]	AR[-]	$E_{V_{\infty}}$ [%]	E_{AR} [%]	AR_{emp}	$E_{AR_{emp}}$ [%]
1.48	Numerical	322	1.40	-	-	1.43	1.96
	Kosior et al. (2012)	346	1.65	6.94	15.15	1.53	-8.06
	Moore (1965)	331	1.58	2.72	11.39	1.46	-8.05
	Duineveld (1995)	350	1.52	8.00	7.89	1.55	1.73
1.58	Numerical	324	1.48	-	-	1.48	-0.27
	Tsao and Koch (1997)	260	1.60	-24.62	7.50	1.26	-21.25
	Moore (1965)	336	1.69	3.57	12.43	1.53	-9.28
	Duineveld (1995)	356	1.63	8.99	9.20	1.64	0.64
2.62	Numerical	272	1.69	-	-	1.66	-1.81
	Zenit and Legendre (2009)	287	1.63	5.23	-3.68	1.80	9.44

Table 5: Comparison of the bubble terminal velocity and aspect ratio obtained numerically (present study) with other benchmarking experimental data.

	Exp	3D	E(3d) [%]	2D	E(2d) [%]
1st	2.583	3.240	-25.416	3.225	-24.816
2nd	1.874	1.861	0.682	1.884	-0.560
3rd	1.560	1.570	-0.640	1.561	-0.089
4th	1.408	1.493	-6.035	1.460	-3.685
5th	1.312	1.421	-8.306	1.422	-8.367
6th	1.252	1.352	-8.001	1.341	-7.155

Table 6: Comparison of the bubble center of gravity at the point of maximum rebound measured from the upper wall for the first six bouncing cycles with air/water mixture and $D_{eq} = 3.3$ mm and Refined mesh.

	Bouncing cycle	thickness [μm]	KE[J]	PE[J]
case II	1st	14.8	6.34E-08	6.72E-09
	2nd	8.60	1.32E-08	3.83E-09
	3rd	6.00	3.00E-09	1.15E-09
	4th	4.80	5.93E-10	8.71E-10
case I	1st	51.9	3.42E-07	2.07E-08
	2nd	24.6	4.35E-08	8.43E-09
	3rd	14.6	3.83E-09	1.07E-08

Table 7: Film minimum thickness and bubble kinetic and potential energy for each bouncing cycle for both $D_{eq} = 1.48$ mm with air/water mixture (case I) and $D_{eq} = 2.62$ mm with air/FluidA mixture (case II).

Highlights:

- A VOF model of bubble impact on a solid surface is compared to experimental data.
- The algebraic VOF method of OpenFOAM is used to solve the two-fluid flow problem.
- Adequate mesh refinement is critical for accurate modelling of the liquid film.
- Static and dynamic contact angle models give similar contact line behaviour.
- The bubble deformation is attributed to a pressure peak in the film region.