VOLUME OF FLUID SIMULATION INVESTIGATIONS ON BUBBLE BURSTING AT A FREE SURFACE

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Abstract
This paper investigates the volume of fluid model in order to simulate bubble bursting at free surface. Transient conservation equations of mass and momentum with consideration of tension and gravitational force effects were solved. The simulation results of bubble rising at stagnant liquid were validated with numerical and experimental results of literature where the agreement was good. A single gas bubble with constant density and viscosity was released in stagnant liquid to reach to a free surface of the gas properties and bursting. The simulations were preformed in a two-dimensional Cartesian coordinate system and indicated that volume of fluid method is a suitable approach in order to simulate collapsing bubbles at free surfaces. However, volume of fluid technique could be developed in order to increase bubble behavior at free surfaces.

Key Words: Bubble bursting, Free surface, Simulation, Two-phase flow, Volume of Fluid.

1. Introduction
Flows with a spatial variation of fluid properties, such as gas–liquid interfaces due to density variation, can be found in many engineering and environmental applications. There are plenty researches in this discipline focuses on subjects such as bubble characteristics, local and average heat transfer measurements, studies of flow regimes and computational fluid dynamics, and mass transfer studies [1,2,3,4]. Although, a tremendous number of studies exist in the literature, bubble behavior is still not well understood due to the fact that majority of these studies are often oriented on only one phase, i.e. either liquid or gas. The main point of interest should be the study of the interaction between the phases, which are in fact intimately linked. In the past several decades a number of different methods have been developed to simulate complex two-phase flow problems. The simulation of the dynamics of gas–liquid involves the solution of the continuity and momentum equations for the two fluids with specified boundary conditions. The description of the free surface offers a particular challenge, which can be dealt with numerically from either the Eulerian or Lagrangian viewpoint. There are three basic approaches commonly employed in the computational fluid dynamics (CFD) for the study of multiphase flows: Eulerian–Eulerian (E–E) method, Eulerian–Lagrangian (E–L) method and direct numerical simulation (DNS) method [5,6,7]. DNS approach is often chosen to study the behavior of formation and rising bubble in multiphase flows.

In order to solve the moving interface problem. There are various methods to project the phase interface position and motion in DNS method and fixed-grid method is widely used due to its efficiency and relative ease in programming. The numerical approaches used to resolve the moving interface problem with fixed, regular grids are improved as the front capturing method. In the front capturing method moving interface is implicitly represented by a scalar-indicator function defined on a fixed, regular mesh point. Among the techniques of front capturing, volume of fluid (VOF) method is designed for two or more immiscible fluids where the position of the interface between the fluids is of interest.

The Volume-Of-Fluid method originally developed by Hirt and Nichols [8] has been the most frequently used approach to simulate free-surface flows. Therefore, it has also received a considerable amount of attention in the study of phase change phenomena. Developed VOF technique with phase change has been employed to simulate two-dimensional film boiling and heat and mass transfer in order to predict liquid evaporation rate [9,10,11], droplet evaporation [12,13] and droplet impacting [14,15] on hot surfaces. The VOF method satisfies the compliance of mass conservation extremely well. The disadvantage of VOF method is that sometimes it is difficult to capture the geometric properties (interface normal and curvature) from the VOF function whose spatial derivatives are not continuous near the interface. Inaccurate calculations of geometric properties lead to unphysical flows around the interface due to imbalance of surface tension force. The VOF method can be used to accurately predict the shape of the interface between the fluids. However, no boundary condition of interface slip is specified in the VOF model; therefore the gas and liquid phases share a common velocity field. Sometimes it is difficult to consider the interaction between two phases, which is the key to successfully describe the flow behavior. In this paper, the volume of fluid numerical approach has been used to simulate bubble collapsing at free surface.

2. Mathematical models

2.1. Governing equations

The compressibility of gas phase is neglected due to (1) the gas velocity is far smaller than the sound velocity and (2) the needed time for obvious change of gas velocity is much longer than the time needed for that sound goes through the characteristic length of flow domain. Continuity and momentum equations for an incompressible Newtonian liquid are as follows:

$$\nabla.\vec{u} = 0 \tag{1}$$

$$\frac{\partial(\rho\vec{u})}{\partial t} + \nabla.(\rho\vec{u}\vec{u}) = -\nabla p + \nabla.\{\mu[\nabla\vec{u} + (\nabla\vec{u})^T]\} + F_s + \rho\vec{g} \tag{2}$$

Where ρ is density of phases, μ is viscosity and F_s is the surface tension force. Volume fraction in VOF model is achieved by solving volume fraction continuity equation of one phase or several phases. As for the q phase, volume fraction continuity equation is:

$$\frac{\partial F_q}{\partial t} + \vec{u}_q.\nabla F_q = 0 \tag{3}$$

The primary phase is not solved by equation (3), primary phase volume fraction calculation is based on the following constraints:

$$\sum_{q=1}^{2} F_q = 1 \tag{4}$$

2.2. Calculation of Fluid Characteristics

The calculating method of density and viscosity of mixing fluid in a computational cell is as follows:

$$\rho(\vec{x},t) = F(\vec{x},t)\rho_l + [1 - F(\vec{x},t)]\rho_g \quad (5)$$

$$\mu(\vec{x},t) = F(\vec{x},t)\mu_l + [1 - F(\vec{x},t)]\mu_g \quad (6)$$

2.3. Continuum Surface Force (CSF) Model

The surface tension force term in Equation (2) is considered by applying the continuum surface force (CSF) model proposed by Brackbill et al. [16]. In this model, the surface tension force is considered to be constant along the surface, and only the forces normal to the interface are considered. The surface tension force at the bubble–liquid interface is expressed as a volume force in the momentum equation using the divergence theorem. This volume force for gas and liquid two-phase is given by:

$$F_s = \sigma \frac{\rho k \nabla F_l}{0.5(\rho_g + \rho_l)} \quad (7)$$

Where $k = \nabla.\hat{n}$, $\hat{n} = n/|n|$, $n = \nabla F_q$.

3. Solution Method and Grid Independency

The finite volume method was used to solve the continuity equation, momentum equation and volume of fluid function equation. The first order upwind scheme was applied to the discretization scheme of the flow equations. This scheme is more stable than the second order upwind scheme and used most often with reasonable accuracy. Pressure–velocity coupling method was the pressure-implicit with splitting of operators (PISO) and also pressure equations were discretized through pressure staggering option (PRESTO) method. The numerical simulations were executed on the software platform of Fluent 6.3 with high performance of 32-core super computing system.

In order to found out grid independency to simulation results, a cylindrical bubble column with 20mm width and 30mm height has been simulated in cartesian coordinate system which is shown in Fig. 1. An initially static bubble with 4mm diameter was released to rise up in stagnant liquid. In order to find out an independent mesh on the solution domain five different mesh sizes were considered. The examined grid sizes were 0.2mm×0.2mm, 0.25mm×0.25mm, 0.3mm×0.3mm, 0.35mm×0.35mm, 0.4mm×0.4mm, and the corresponding numbers of grid points were 3825, 4902, 6700, 9600, 15150 ,respectively. Furthermore, the time step in these simulations was set as 0.0001 second.

Simulation results of single bubble rising at three different time steps at 0, 0.025 and 0.05 second are shown in Fig .2. The profiles of single bubble rising with different grid sizes at time of 0.05s are shown in Fig .3. In order to achieve mesh independency vertical velocities at y direction on the center line ($x = 0, 0.005 \leq y \leq 0.015$) at time of 0.05s with all different meshes was plotted and considered which is shown in fig .4. It is worth noting that in all figures, blue fluid is liquid phase and red fluid is gas phase. Consequently, the grid size of 0.25mm was considered as independent grid with high accuracy in this 2D simulation.

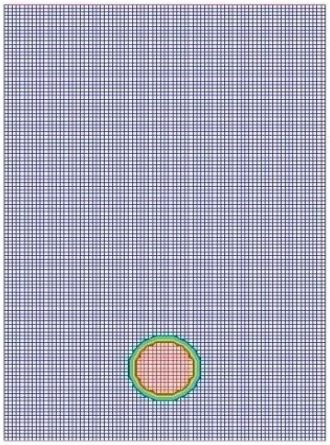


Figure 1: The solution area of rising single bubble and initial released bubble made with 9600 meshes (mesh size 0.25mm)

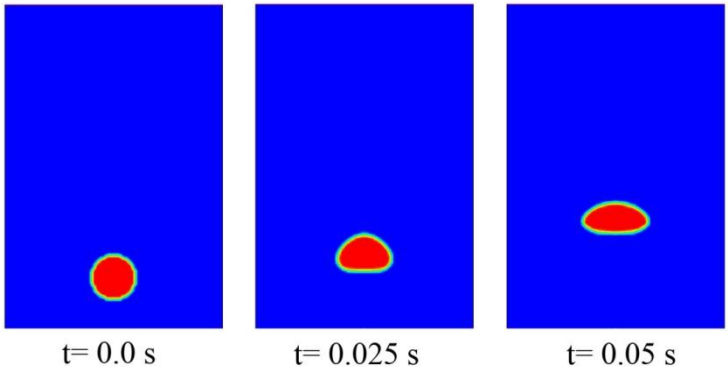


Figure 2: Simulation results of single bubble with 4mm diameter rising at three different time steps with 9600 meshes

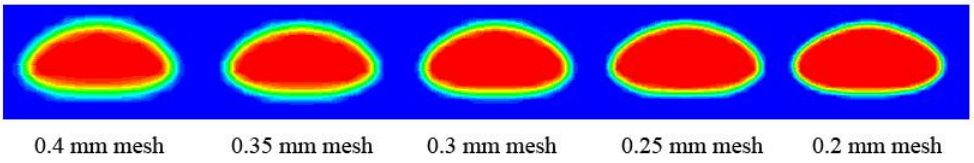


Figure 3: The profiles of single bubble rising with different grid sizes at time of 0.05s

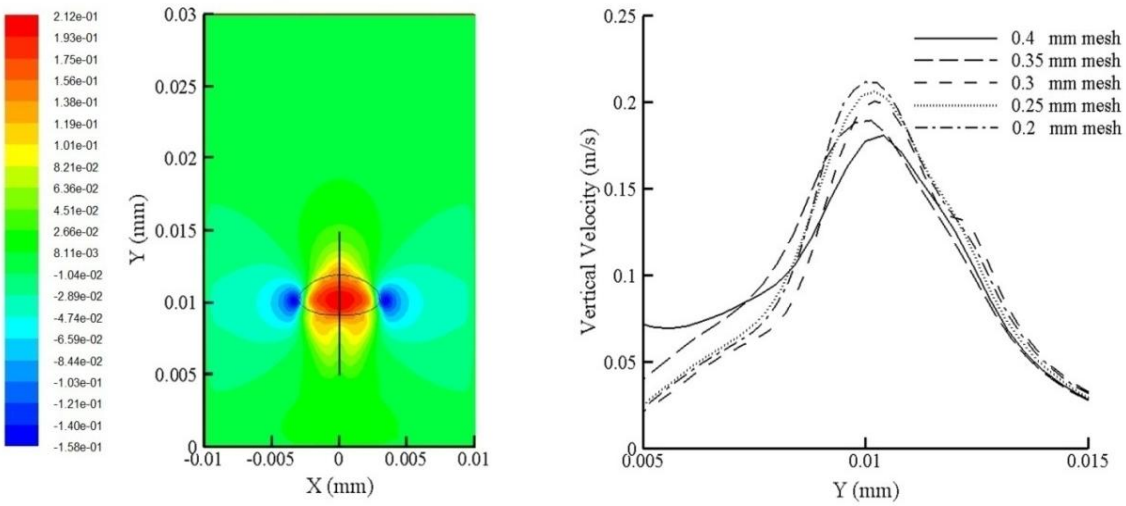


Figure 4: Contour and the plot of vertical velocities at y direction on the center line $x = 0, 0.005 \leq y \leq 0.015$ () with various meshes at t=0.05s

4. Simulation verification

In present research, two-dimensional simulation in cartesian coordinate system was investigated and compared with experimental and three-dimensional numerical studies. Simulation results of bubble formation and rising motion from an orifice with 1mm diameter and high orifice gas velocity of 3.0 m/s was compared with Yujie et al. [17] numerical and experimental study which are shown in Fig. 5. Yujie et al. [17] investigated three-dimensional numerical simulations on bubble formation in bubble columns using the volume of fluid (VOF) model on the software platform of Fluent and they also surveyed bubble behavior experimentally.

All present computations were performed through physical characteristics of gas and liquid phases which are listed in table 1. Bubble diameter and rise velocity are also listed in Table 2. It is found from Fig. 5 and table 2 that in two-dimensional simulation bubble velocity and bubble diameter had 8 and 9 percent error with experimental data, respectively, also there are 3.5 and 7 percent error with three-dimensional numerical simulation. Consequently, there are reasonable agreements between experiments and simulations of bubble behavior in the process of bubble generation and rising motion.

Table 1: properties of gas and liquid phases in the simulations

$\rho_g(kg/m^3)$	$\rho_l(kg/m^3)$			$\sigma_l(N/m)$	$d_o(mm)$
1.225	9.982e2	1.789e-5	1.0e-3	7.28e-2	1.0

Table 2: Comparison of present simulations with experimental and numerical studies with 1.0mm orifice diameter and $v_g = 3\ m/s$.

	Bubble diameter (mm)	**Bubble velocity (m/s)**
Experiments[17]	7.00	0.275
3D simulation[17]	7.12	0.262
2D simulation	7.65	0.253

5. Bubble Bursting at a Free Surface

Gas bubble bursting at free surface finds essential applications in health problems such as in cell damage process, in transfer of mass and various contaminants for chemical and nuclear industry and in the geophysical field. The problem under consideration in this study was a single gas bubble of constant density and viscosity rising through a liquid of constant density and viscosity, in a gravitational field with a constant acceleration due to gravity and then bursting at a free surface. In order to simulate a spherical bubble collapse at free surface through the VOF method, a mesh zone consists of 120×120 cells was considered which half of it was defined as liquid phase and other as gas phase. A gas phase spherical bubble with 4mm diameter was released in liquid phase at 4mm distance of free surface. Computational domain with cartesian coordinate system (x, y) and grade zone of bubble rising process are shown in Fig. 6 for this present work.

The shape of a single bubble results from a balance between two opposing effects: the buoyancy F_B, of the order of $\rho g \pi R^3$, which tends to make it emerge from the free surface and the capillary force F_C inside the hemispherical thin liquid film, of the order of $(\gamma/R)\pi R^2 = \gamma\pi R$, which tends to maintain the bubble below the surface, where γ and ρ are respectively the

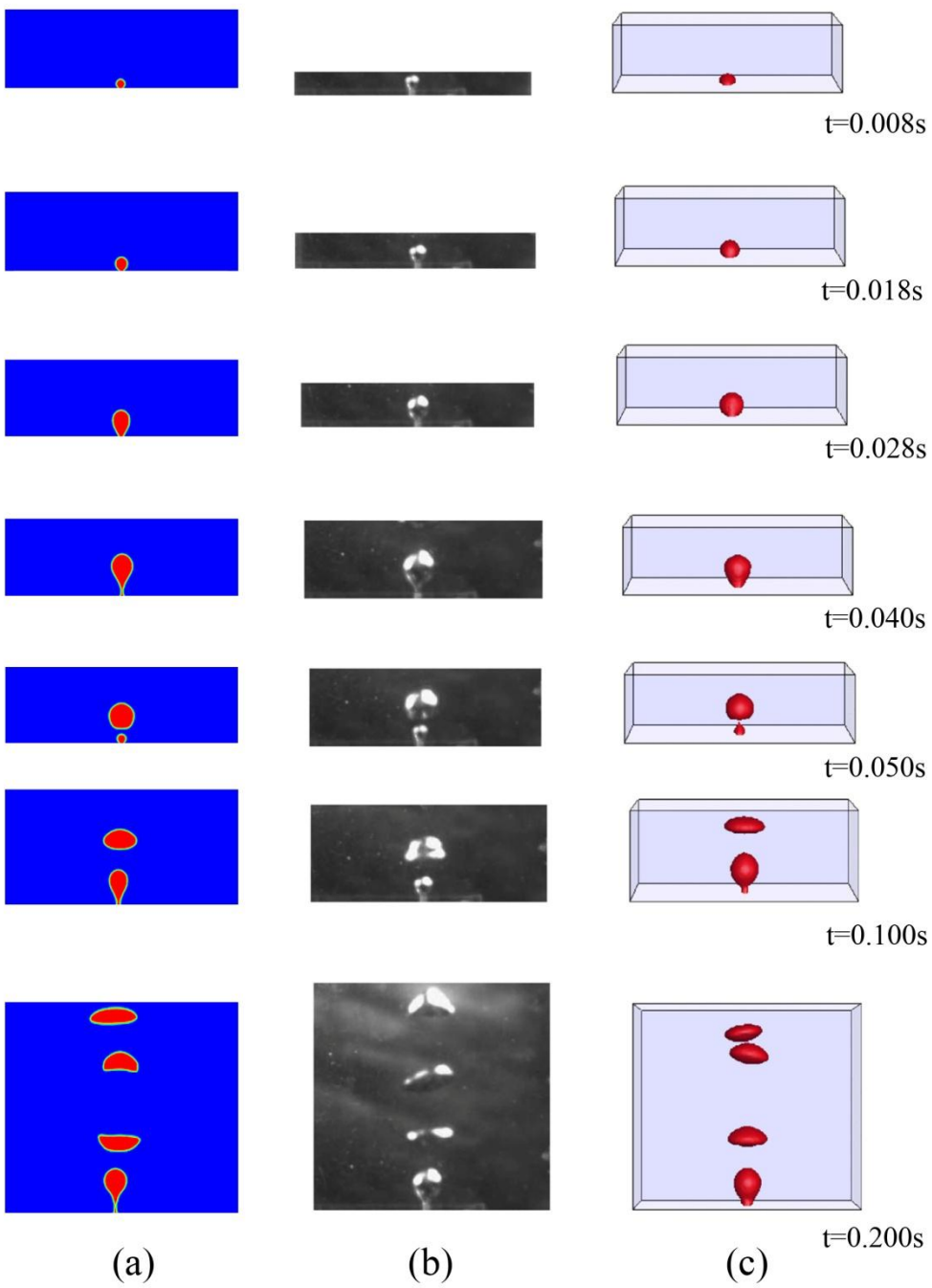
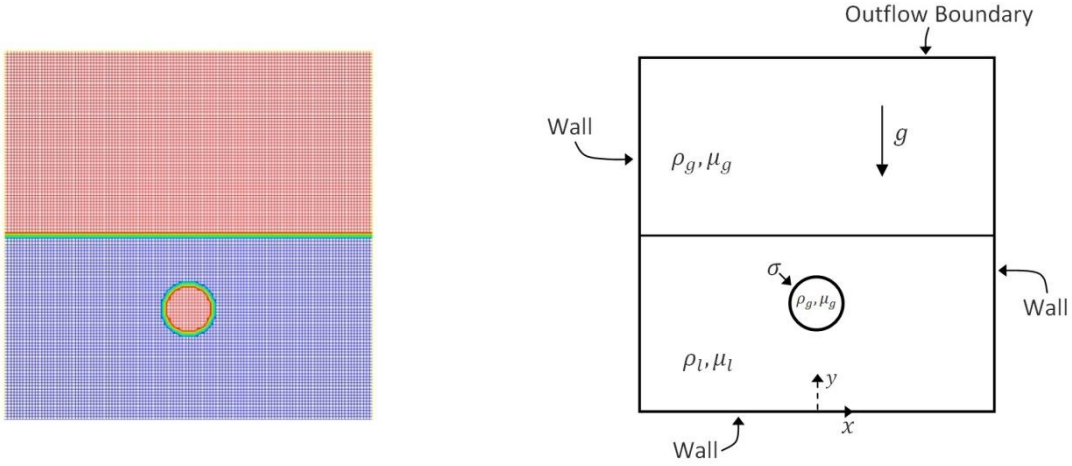


Figure 5: Comparison of present simulations with experiments and simulations of bubble formation from an orifice of 1.0 mm diameter and rising motion when $v_g = 3\ m/s$. (a) 2D simulation, (b) experimental observation [17] and (c) 3D simulations [17]

liquid surface tension and the liquid density [18]. At the free surface, since bubble's radii are significantly smaller than the capillary length, the liquid films of bubble caps progressively get thinner due to capillary drainage. When the liquid film of a bubble cap reaches a critical thickness, it becomes fragile and finally ruptures. Simulated results of single bubble rising and collapsing through the volume of fluid method are given in Fig. 7 which are compared with simulation results of I. Chakraborty et al. [20] using a coupled level-set and volume-of-fluid (CLSVOF) method. The simulation results reveal good agreement with literature [19, 20]. We have been able to compute the evolution history of a gas bubble of diameter 4 mm

bursting to an air-water interface. However, the volume of fluid method should be developed in order to simulate more accurately bubble collapsing at free surface.



(a) (b)

Figure 6: (a) Grid zone and (b) computational domain and boundary condition, to investigat single bubble collapsing process at free surface

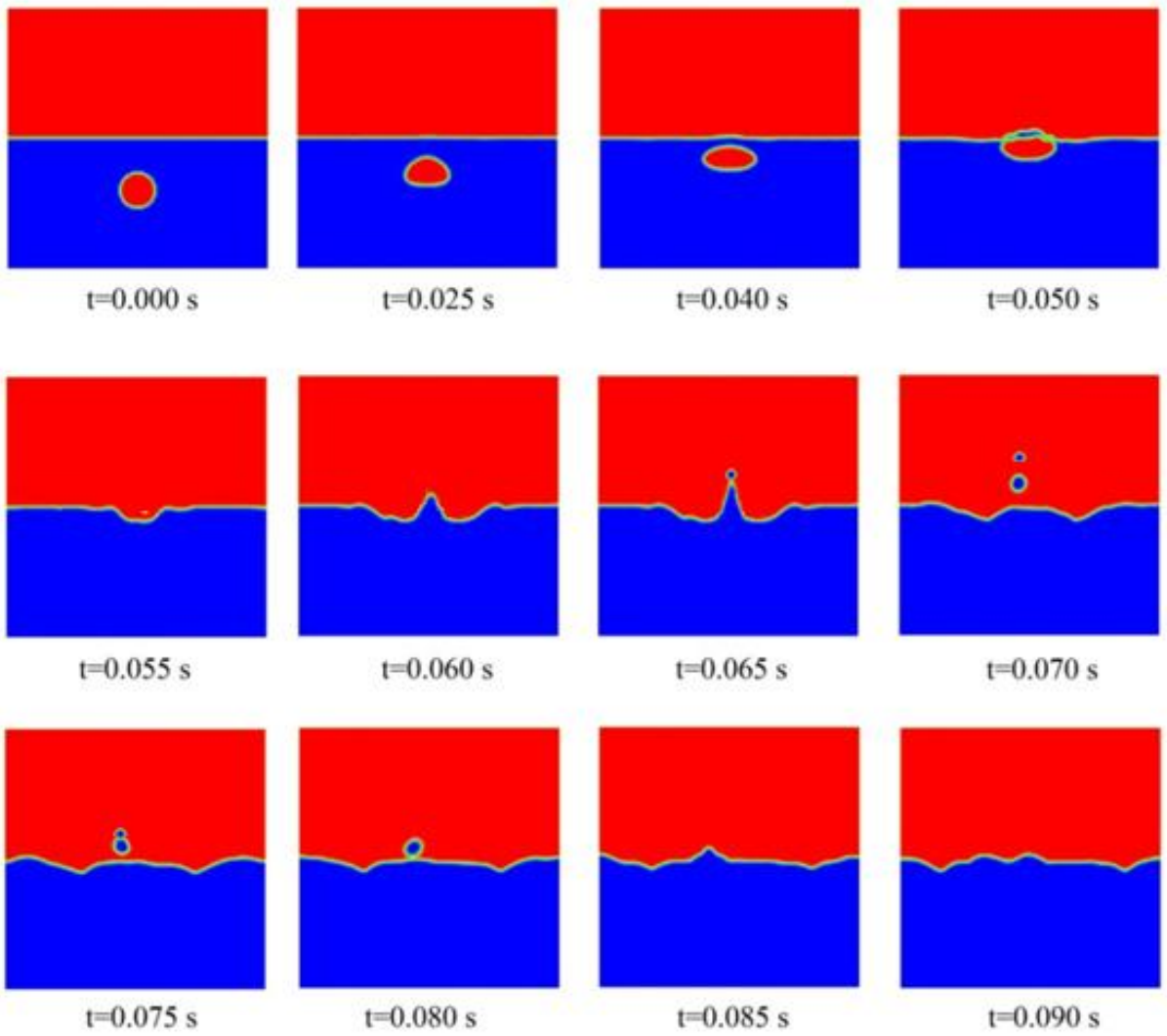


Figure 7: Simulation of bubble collapsing at free surface

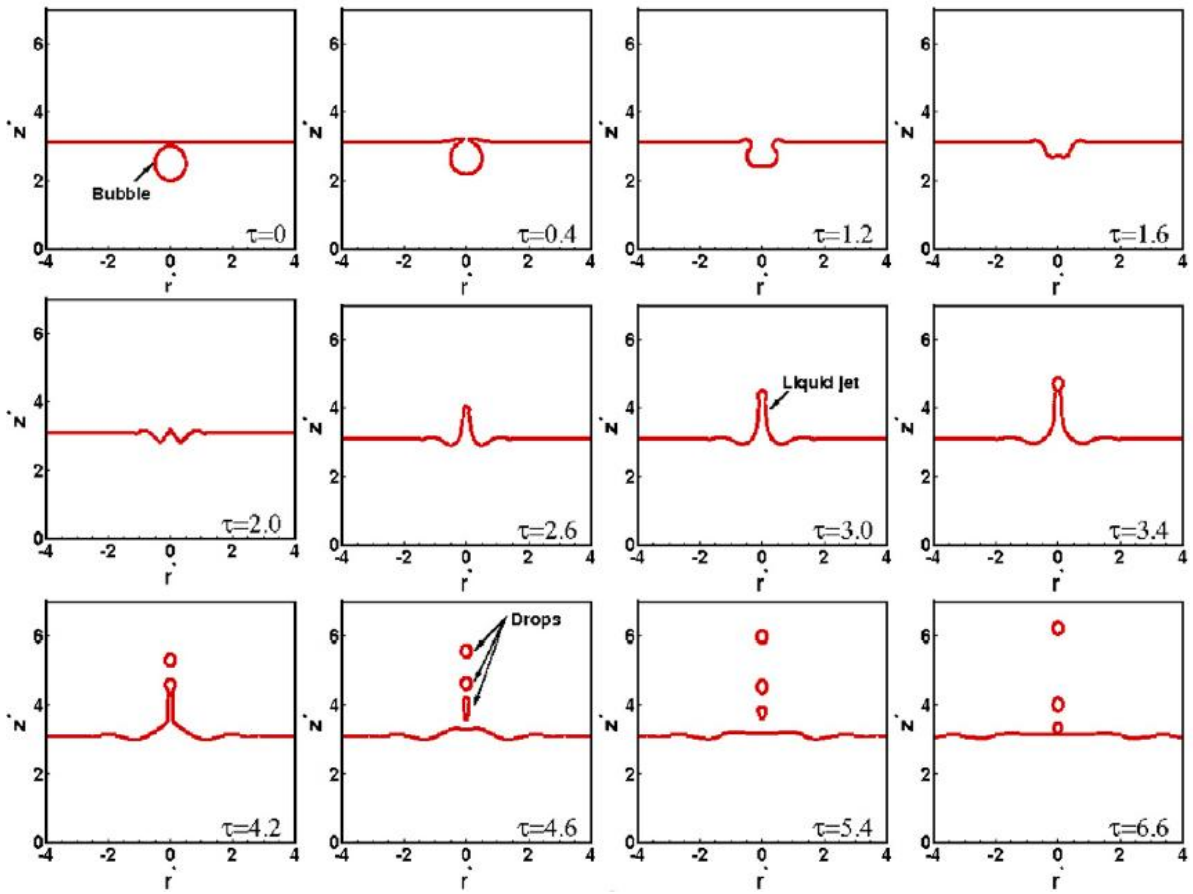


Figure 8: Time sequence of a gas bubble of 6mm diameter bursting at a air-water interface resulting formation of liquid jet and small drops using our CLSVOF method [20].

6. Conclusion

Numerical simulations of two-phase incompressible flows have been performed using volume of fluid method (VOF). The VOF approach was employed to simulate bubble busting at free surface. It was found that the predicted results of bubble bursting were in good agreement with literature. Nevertheless, VOF method could be developed and coupled with other techniques such as level set method in order to increase the surface curvature accuracy. Moreover, the VOF method has the drawback of artificial coalescence of bubbles when the mutual distance is lower than a computational cell size. Hence, further work is needed to overcome these limitations. The VOF method satisfies the compliance of mass conservation extremely well and also the disadvantage of this method is that sometimes it is difficult to capture the geometric properties (interface normal and curvature) from the VOF function whose spatial derivatives are not continuous near the interface.

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