

# Study of Bubble Dynamics and Free Liquid Surface Mixing in a Rectangular Container Having Ullage Area with Double Gas Inlets



Sarath Raj and J. S. Jayakumar

**Abstract** In this work, the Volume of Fluid (VOF) [1] method is used to study bubble dynamics and collapse of bubbles on free surface in a rectangular domain with double gas inlets. The simulation is done by using open-source CFD software OpenFOAM-3.0.1. The conservation equations for mass and momentum, which incorporates the influence of surface tension and gravity, are solved by using PIMPLE algorithm. The physical model for the simulation process is a 2D rectangular domain with a width of 50 mm and height of 100 mm. In order to study the collapsing of the bubble on the surface and free liquid surface mixing, an ullage area of 15% was considered within the domain. The numerical computation was performed with multiphase solver *interFoam*. Modeling of the geometry, meshing and setting the boundary conditions were done, using the OpenFOAM software. The simulation results were compared with the available literature results and found that the bubble formation and dynamics are in good agreement. The behaviors of gas bubbles emanating from two adjacent orifices at different gas velocities are studied. Mixing behavior in the bulk liquid due to bubble formation under different inlet gas velocities was also numerically investigated. The impact of surface tension and density of bulk liquid on collapsing of the bubble on the free liquid surface is investigated numerically.

**Keywords** Bubble dynamics · *interFoam* · OpenFOAM · VOF · CFD

## 1 Introduction

Gas–liquid bubble columns are extensively used as reactors and multiphase contactors in chemical, biochemical, petrochemical industries, and in various other engineering applications. It has numerous advantages, which can be explained in terms

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of higher heat–mass transfer rates, efficient interphase interaction, compactness, low operating and maintenance cost, etc. Even though a large number of studies prevail in the literature, bubble column studies are still not well established because the majority of these studies were often carried out on only one phase, i.e., either gas or liquid. However, in bubble columns, the primary focus should be given to the interaction between the different phases, which are in fact mutually linked. Bubble performance is crucial in defining the fluid characteristics in bubble columns.

In bubble columns, due to high density and viscosity ratios, the motion of bubbles can be very intricate and also is very problematic so as to estimate an accurate mathematical model that can be used to compute the bubble rise velocity in various transport properties. In the past, numerous periods and numerous techniques were developed to simulate complex two-phase flow problem. Denoij et al. [2] studied the time-dependent behavior of the large gas bubble by using volume tracking method. The volume tracking method is based on Volume of Fluid concept. With the help of volume tracking model, the authors studied the formation and rising behavior of skirted bubble, spherical cap bubble. Shimizu et al. [3] carried out experimental analysis in bubble column reactor and based on that model for bubble break up and agglomeration, they studied the gas holdup and gas–liquid mass transfer phenomena. Arsam et al. [4] measured the mass transfer coefficient and bubble size distribution in large-scale industrial bubble column reactor for CO, N<sub>2</sub>, H<sub>2</sub>, and CH<sub>4</sub> in two organic mixtures solids in a wide pressure range, superficial gas velocities, and solid concentration. From the experimental analysis, the authors found that the values of mass transfer coefficient depend on bubble size distribution. Andrzej et al. [5] studied bubble dynamics using Computational Fluid Dynamics (CFD) software. For tracking the liquid interface in 2D and 3D domain, the authors used momentum balance equation coupled with Volume of Fluid algorithm. Ammar et al. [6] investigated the behavior of bubbles in a bubble column by using the VOF model. The authors compared the results of both commercial and Open-Source Solver with experimental results. From the analysis, it was found out that the numerical results showed a better prediction of the gas bubble hold up in bubble column, compared with experimental results. Han et al. [7] numerically studied the impact of surface tension on bubble behavior of a spherical bubble rising in a stationary liquid using VOF method. For the simulation for bubble dynamics, the authors used the gas–liquid density ratio as 0.001 and found out that there exist four critical Weber numbers which differentiate five different kinds of bubble behaviors. Ma et al. [8] carried out a numerical simulation to study the bubble dynamics by using Fluent 6.3. For the simulation, the authors used Volume of Fluid method and Continuum Surface Force model. The authors studied the effect of physical properties such as surface tension, liquid viscosity, density, and orifice size on various bubble behaviors. Peyman et al. [9] carried out a numerical simulation to examine the formation and motion of bubbles in bulk liquid by using VOF method. For the numerical investigation, the authors used FLUENT 6.3. For simulating gas–liquid interface, the pattern in VOF method conservation of mass and momentum equations were used. The authors studied the effect of fluid physical properties and orifice diameter in bubble behavior, detachment time and found out bubble detachment time is linear function of surface tension. Tariqul et al.

[10] investigated the effect of inlet gas velocity and Reynolds number on bubble formation in viscous liquid using VOF-CSF method in CFD. The study has verified the capability of CFD to predict the bubble velocity, bubble shape, and detachment time was in good agreement compared to experimental analysis. Kang et al. [11] carried out an experimental analysis in pressurized bubble column of diameter 0.152 and height of 2.0 m and they investigated the bubble distribution and its effects on the gas–liquid mass transfer. Wang et al. [13] numerically investigated the phenomenon of bubble agglomeration, considering two droplets with different temperature. For the simulations, the authors used VOF method and for describing the effects of interfacial tension force the Continuum Surface Stress model was used.

In the present work, the VOF [1] technique is applied in the simulation of bubbling characteristics and collapse at free liquid surface. The simulation dealt with bubble behavior in a 2D rectangular domain with double orifice of small diameters in contrast to the single orifice simulations carried out earlier using other CFD tools. So far, no studies have been reported on bubble dynamics and collapse at free surface in a rectangular container with double orifices using OpenFOAM. The time for bubble detachment, average bubble diameter, and the agglomeration and mixing rates of bubbles are deliberately scrutinized by utilizing computer simulations.

## 2 Governing Equations

The continuity and momentum equations for two-phase flow fluid problems are written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (1)$$

$$\frac{\partial(\rho \vec{v})}{\partial t} + \nabla(\rho \vec{v} \vec{v}) = -\nabla p + \nabla[\mu(\nabla \vec{v} + \vec{v})] + F_s + \rho \vec{g} \quad (2)$$

### 2.1 VOF Model

In the VOF scheme, the fluids share a solitary set of momentum and volume fraction equations. Hence, each computational grid is traced along the entire domain. VOF methodology depends on the assumption that the fluid phases do not interpenetrate each other and uses the function  $F(x, y, t)$ , whose value is 1 at any point occupied by pure liquid, 0 for pure gas and the value ranges between 0 and 1 for gas–liquid composition.

$$F = \frac{\text{Volume of fluid in unit}}{\text{Volume of unit}} \quad (3)$$

$$F = \begin{cases} 0 & \text{In bubble} \\ 0 < F < 1 & \text{Interface} \\ 1 & \text{In liquid fluid} \end{cases} \quad (4)$$

The transport equation of fluid volume function is

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + (\vec{v}\nabla)F = 0 \quad (5)$$

## 2.2 Interface Reconstruction Techniques

Various methods are available for solving fluid volume functions like the donor–acceptor, FLAIR, SLIC, and PLIC methods [7, 8]. In Piecewise Linear Interface Calculation (PLIC) method, the interface fluid transport is incorporated in detail and reconstruction details are moderately accurate. Therefore, the PLIC method is applied here for the reconstruction of fluid interface [7, 8].

## 2.3 Continuum Surface Force (CSF) Model

The CSF model is utilized for calculating the surface tension force in the liquid–gas interface by combining the volumetric force equation and momentum equation [7, 8].

$$F_S = \sigma \frac{\alpha_l \rho_l k_v \nabla \alpha_v + \alpha_v \rho_v k_l \nabla l}{0.5(\delta_v + \delta_l)}$$

where  $k_l = \frac{\nabla \alpha_l}{|\nabla \alpha_l|}$   $k_v = \frac{\nabla \alpha_v}{|\nabla \alpha_v|}$

## 3 Validation

For validating the methodology used in the present study, the work of Ma et al. [8] was considered. The comparison of bubble diameter with inlet gas velocity was investigated. It was observed that with an increase in inlet gas velocity, the bubble average diameter increases, as shown in Fig. 1. The results of the present study are in good agreement with Ma et al. [8] and the relative error was within 5%.

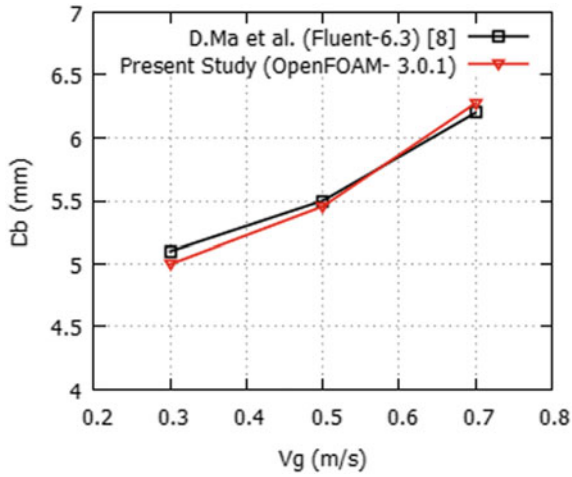


Fig. 1 Bubble diameter versus inlet gas velocity, orifice diameter  $D_o = 0.5$  mm

### 4 Analysis

In the present study, a rectangular domain of 50 mm width and 100 mm height is considered. Figure 2a shows the geometry depiction and dimensional details of a rectangular container with 15% ullage area. The grid is shown in Fig. 2b. An enlarged view of the rectangular region near the orifice is shown in Fig. 2c. Finite

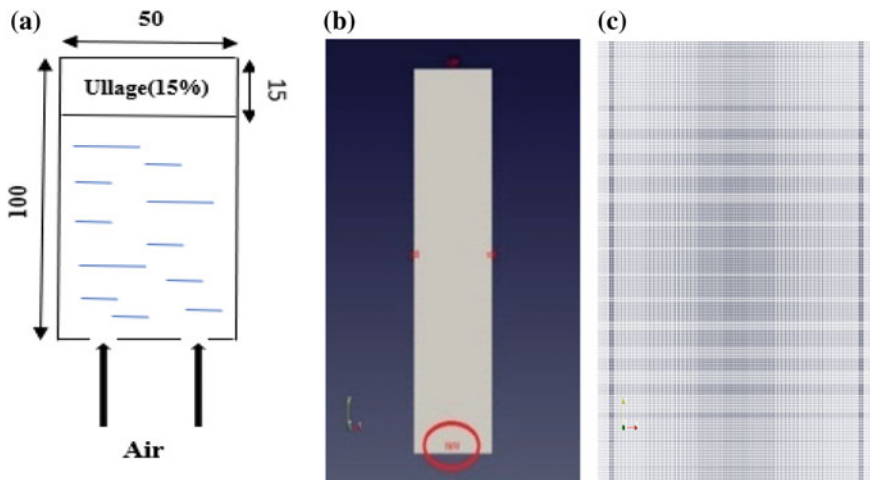


Fig. 2 a Rectangular domain with double inlets and 15% ullage area. b Computational model of rectangular domain. c Enlarged view near the inlet orifice

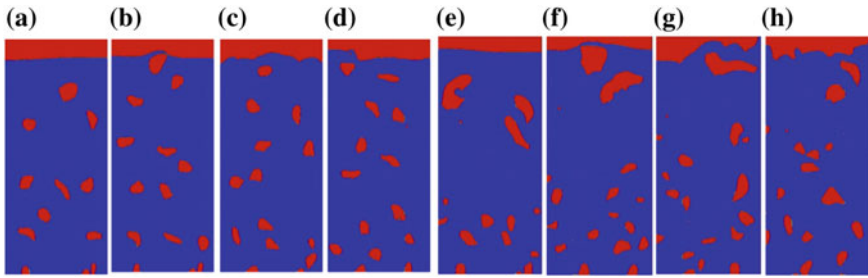
Volume Method (FVM) is used for the discretization of continuity and momentum equation. PIMPLE algorithm is employed to convert PDE to a system of algebraic equations and is solved concurrently. The Piecewise Linear Interface Calculation (PLIC) method is applied here for the reconstruction of fluid interface [7, 8].

Numerical computations are performed with well-known multiphase solver `interFoam`. For these simulations, a small time step of the order 0.1 ms is considered. The gas inlets are defined as velocity inlets. The walls are defined as no-slip. For checking the dependency of a number of cells on the analysis, five ranges of cell numbers are used. The results show that a representative accuracy can be attained in bubble behavior simulation with cell number  $9.00e+05$  and the precision did not improve even if a higher cell number used [12].

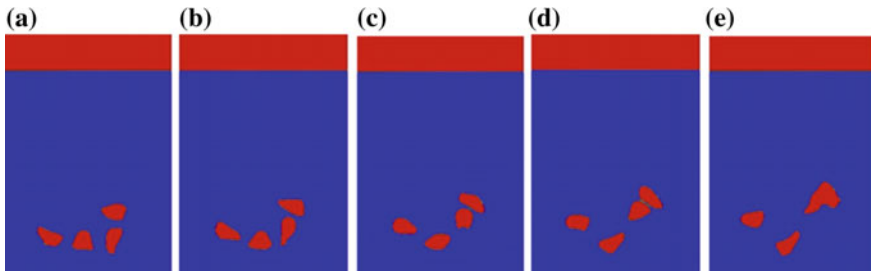
## 5 Results and Discussion

### 5.1 Influence of Inlet Gas Velocity on Bubble Behavior and Free Liquid Surface Mixing

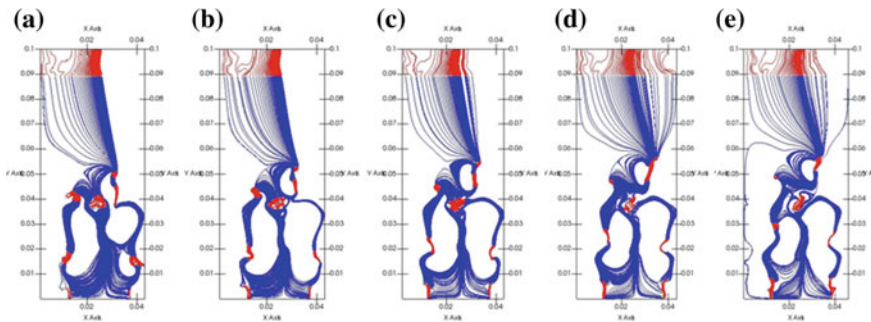
The influence of inlet gas velocity on bubble detachment time, diameter of bubble, and free liquid surface mixing are numerically simulated and the results are shown in this section. The phase contours (Fig. 3) show the influence of inlet gas velocity in free liquid surface collapsing and bursting. In which the blue part shows the liquid phase and the red portion shows the air bubble. The liquid surface gets more deformed with the increase in inlet gas velocity and is clearly shown in Fig. 3e–h. At the initial stage, the bubble develops and grows but the gas bubble neck still remains in contact with the orifice mouth. The surface tension force plays an important part at this moment. When the buoyancy force on the bubble overrules the liquid drag force, bubble gets detached from the orifice and finally gets deformed. The process is repeated for the consecutive bubbles. Figure 4 shows the void fraction contours for bubble coalescence and the position changes of bubbles along the vertical direction of the rectangular domain during agglomeration at inlet gas velocity of 0.5 m/s. It is clear that velocity of the first bubble is lower than that of the trailing bubbles. This means that the trailing bubbles accelerates more under the wakening effect of the first bubble and thus the distance between the first leading and second trailing bubble get reduced and ultimately with the increment in time the bubbles get agglomerated to form a single larger bubble. Streamline contours are plotted to study the disturbance pattern of the wakes behind the leading bubble. Figure 5 shows the streamlines around the bubble when orifice diameter is 0.5 mm and inlet gas velocity is 0.5 m/s. The vortices created at either end sides of the rising bubble are also shown in Fig. 5. Figure 6a shows the position changes of bubbles along the vertical direction of the rectangular domain during agglomeration. It can be observed that the upper first bubble gets deformed at a much faster rate than the lower rising bubble. This is because of the



**Fig. 3** Bubble behavior for various inlet gas velocities when  $D_o = 0.5$  mm, **a**  $t = 0.62$  s, **b**  $t = 0.72$  s, **c**  $t = 0.82$  s, **d**  $t = 0.92$  s, **a-d**  $V_g = 0.5$  m/s, **e**  $t = 0.62$  s, **f**  $t = 0.72$  s, **g**  $t = 0.82$  s and **h**  $t = 0.92$  s, **e-h**  $V_g = 0.7$  m/s



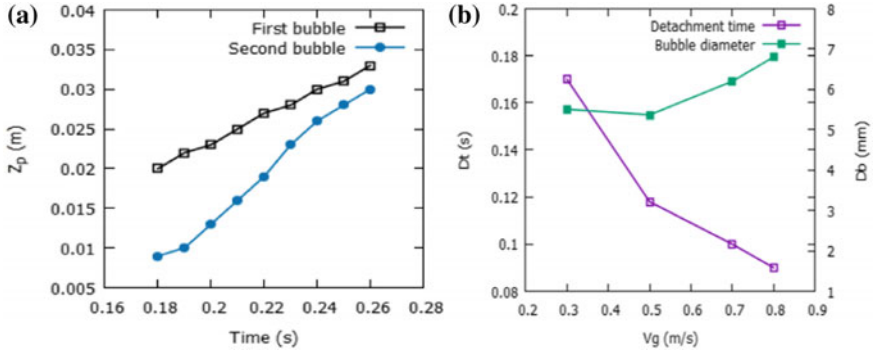
**Fig. 4** Bubble agglomeration process of two bubbles in the bubble column when  $D_o = 0.5$  mm, **a**  $t = 0.40$  s, **b**  $t = 0.41$  s, **c**  $t = 0.42$  s, **d**  $t = 0.43$  s, **e**  $t = 0.44$  s, **a-e**  $V_g = 0.5$  m/s



**Fig. 5** Comparison of the streamlines around the bubble during bubble coalescence, when  $D_o = 0.5$  mm, **a**  $t = 0.40$  s, **b**  $t = 0.41$  s, **c**  $t = 0.42$  s, **d**  $t = 0.43$  s, **e**  $t = 0.44$  s, **a-e**  $V_g = 0.5$  m/s

fact that the upper first bubble flows through the dormant liquid, while the lower travels through the wake region left behind the upper leading bubble.

A lower drag force is created for the lower bubble due to the wake left behind the upper bubble. Hence, the relative distance between two bubbles gets decreased with



**Fig. 6** **a** Vertical position change of bubbles during agglomeration. **b** Variation in bubble detachment time and diameter with respect to different inlet gas velocity

**Table 1** Transport properties of bulk liquid used for the study of the effect of surface tension on bubble behavior [8]

$\sigma_1$ (N/m)	$\mu_1$ (Pa s)	$\rho_l$ (kg/m <sup>3</sup> )
$4.82 \times 10^{-2}$	$1.005 \times 10^{-3}$	1003.8
$5.38 \times 10^{-2}$	$1.005 \times 10^{-3}$	1006.2
$6.93 \times 10^{-2}$	$1.005 \times 10^{-3}$	1002.2
$7.28 \times 10^{-2}$	$1.005 \times 10^{-3}$	998.2

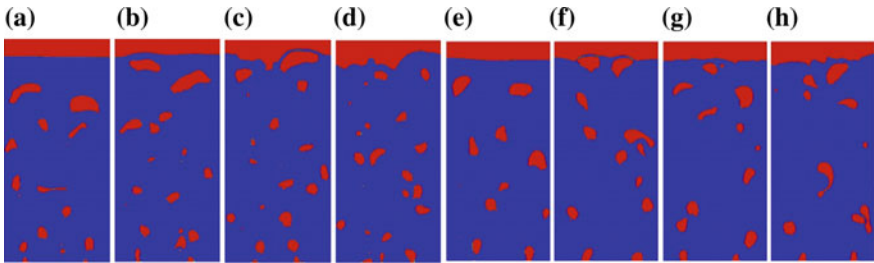
time and is clearly shown in Fig. 6a. The bubble agglomeration causes turbulence in the bulk liquid and microbubbles are formed in the vicinities of bubble fusion.

Free liquid surface collapsing depends on bubble detachment time as well as the bubble diameter. Figure 6b shows the variation in time of detachment and bubble diameter with different inlet gas velocity. It is clear from the figure that bubble diameter increases with increase in inlet gas velocity. But detachment time shows a downward trend with the increment in gas velocity hence bigger and more number of bubbles was formed and bubble rises near to the ullage area which causes the free liquid surface to be deformed more.

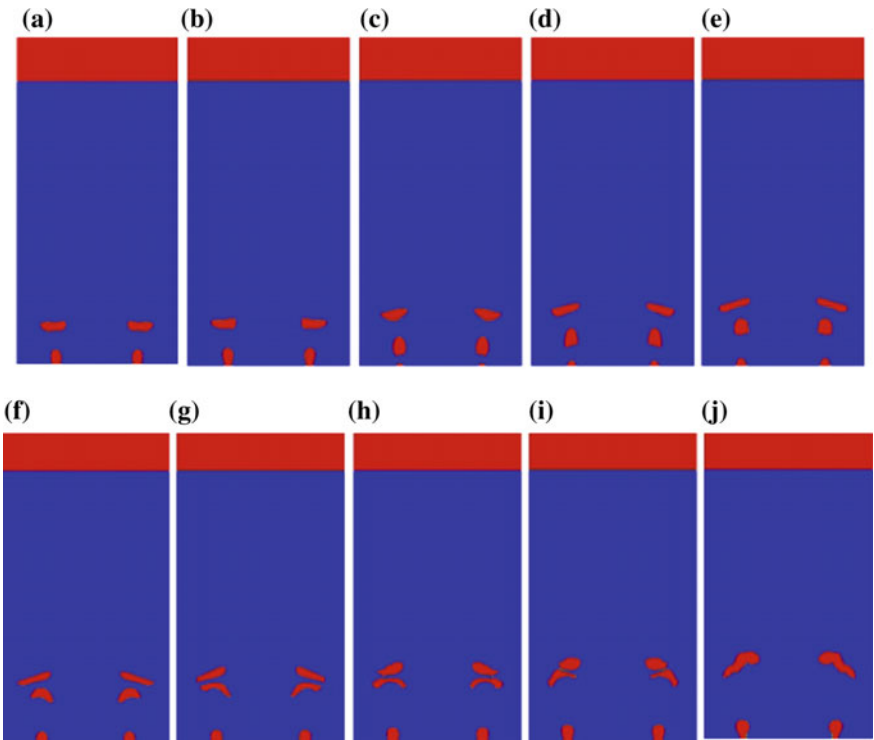
### 5.2 Influence of Surface Tension on Bubble Behavior and Free Liquid Surface Mixing

The impact of surface tension force of bulk liquid on free liquid surface deformation due to bubbling is shown in Fig. 7. Figure 8 shows the void fraction contours for bubble coalescence and the position changes of bubbles along the vertical direction of the rectangular domain during agglomeration at a surface tension value of 0.0538 N/m. The transport properties used to scrutinize the surface tension effects in bubble behavior are enumerated in Table 1.

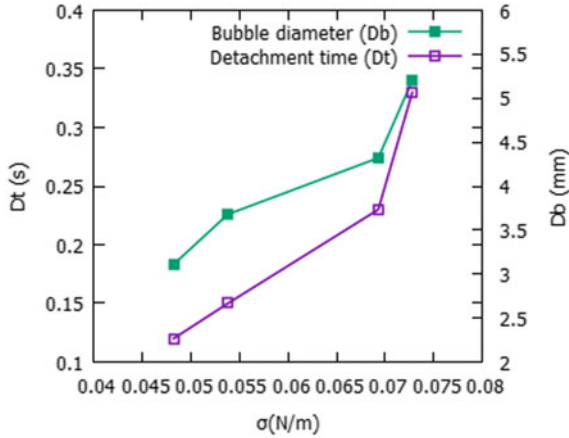




**Fig. 7** Effect of surface tension on free liquid surface collapsing when  $D_o = 0.5$  mm, **a**  $t = 0.68$  s, **b**  $t = 0.78$  s, **c**  $t = 0.88$  s, **d**  $t = 0.98$  s, **a-d**  $V_g = 0.9$  m/s,  $\sigma_1 = 0.0538$  N/m, **e**  $t = 0.68$  s, **f**  $t = 0.78$  s, **g**  $t = 0.88$  s, **h**  $t = 0.98$  s, **e-h**  $V_g = 0.9$  m/s,  $\sigma_1 = 0.0728$  N/m



**Fig. 8** Bubble agglomeration process of two bubbles in the bubble column when  $D_o = 0.5$  mm, **a**  $t = 0.14$  s, **b**  $t = 0.15$  s, **c**  $t = 0.16$  s, **d**  $t = 0.17$  s, **e**  $t = 0.18$  s, **f**  $t = 0.19$  s, **g**  $t = 0.20$  s, **h**  $t = 0.21$  s, **i**  $t = 0.22$  s, **j**  $t = 0.23$  s, **a-j**  $V_g = 0.9$  m/s,  $\sigma_1 = 0.0538$  N/m



**Fig. 9** Variation in bubble diameter and detachment time with respect to different surface tension forces

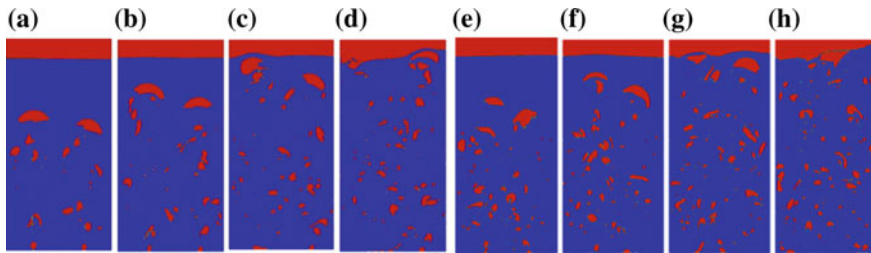
From Fig. 8, it is clear that the velocity of the first bubble is lower than that of the trailing bubbles. This means that the trailing bubbles accelerates more under the wakening effect of the first bubble and thus the distance between the first leading and second trailing bubble get reduced and ultimately the bubbles get agglomerated to form a single larger bubble. The free liquid surface deformation rate depends on bubble detachment time and bubble diameter which is shown in Fig. 9. As the surface tension value is increased, the detachment time increases and bubbles get detached from the orifice mouth at slower rate hence more amount of air is entrapped within the gas bubbles. Therefore, average bubble diameter increases with increase in surface tension of the bulk liquid. At higher values of surface tension, due to the increment in the detachment, timeless number of the bubble are available at the top end near to the ullage area which is clear from Fig. 7. This leads to less turbulence effect and hence collapsing rate of free liquid decreases with increase in surface tension.

### ***5.3 Influence of Density of Bulk Liquid on Bubble Behavior and Free Liquid Surface Mixing***

Formation of a single bubble was numerically simulated in a rectangular 2D bubble column with 15% ullage area in which air is bubbled into liquid water through two inlets. Variation of bulk liquid density has a substantial impact on bubble behavior. The transport properties used in order to scrutinize the density effects in bubble behavior and liquid surface mixing are enumerated in Table 2. The numerical results of bubbling behavior at two different liquid density values equal to 998.2 and 1500 kg/m<sup>3</sup> are shown in Fig. 10. From the contours, it is observed that bub-

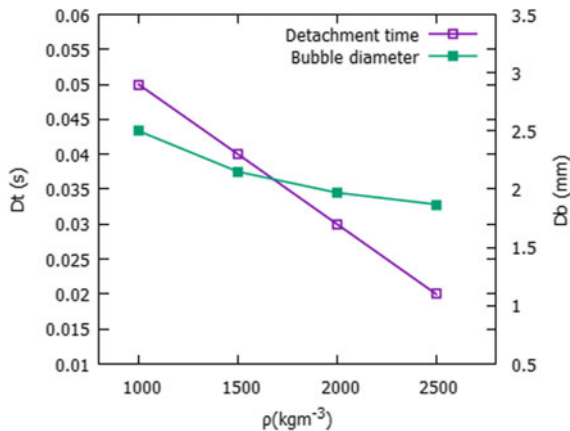
**Table 2** Transport properties of bulk liquid used for the study of the effect of density on bubble behavior [8]

$\rho_l$ (kg/m <sup>3</sup> )	$\mu_l$ (Pa s)	$\sigma_1$ (N/m)
998.2	$1.005 \times 10^{-3}$	$7.28 \times 10^{-2}$
1500	$1.005 \times 10^{-3}$	$7.28 \times 10^{-2}$
2000	$1.005 \times 10^{-3}$	$7.28 \times 10^{-2}$
2500	$1.005 \times 10^{-3}$	$7.28 \times 10^{-2}$



**Fig. 10** Effect of density on free liquid surface collapsing when  $D_o = 0.5$  mm, **a**  $t = 0.65$  s, **b**  $t = 0.75$  s, **c**  $t = 0.85$  s, **d**  $t = 0.95$  s. **a–d**  $V_g = 0.25$  m/s,  $\rho_l = 998.2$  kg/m<sup>3</sup>, **e**  $t = 0.65$  s, **f**  $t = 0.75$  s, **g**  $t = 0.85$  s, **h**  $t = 0.95$  s, **e–h**  $V_g = 0.25$  m/s,  $\rho_l = 1500$  kg/m<sup>3</sup>

ble behavior is influenced by bulk liquid density to a greater extent. Comparing Fig. 10a–d with 10e–h, it can be concluded that increase in liquid density augments the bubbling frequency because a number of bubbles are formed with density value 1500 kg/m<sup>3</sup>, i.e., increase in liquid density increases the frequency of bubbling. The bubble agglomeration causes turbulence in the bulk liquid and microbubbles are



**Fig. 11** Variation in bubble diameter and detachment time with respect to different density values of bulk liquid

formed in the localities of bubble fusion. The influence of bulk liquid density on diameter and detachment time of bubble is shown in Fig. 11.

From Fig. 11, it is clear that the bubble diameter and detachment times are getting reduced considerably with the upturn of liquid density at constant inlet gas velocity. This is because high liquid density increases bubble buoyant force, which makes the bubble to detach early. The coalescence rate and free liquid surface mixing rate also increases because more number of bubbles was formed at high values of liquid density.

## 6 Conclusions

The Volume of Fluid (VOF) method was used to numerically investigate the bubble formation, dynamics and free liquid surface mixing in a rectangular domain with double inlets. The numerical investigation was carried out by using the software `OpenFOAM-3.0.1`. Compared to other methods the VOF method has less computational intricacy, higher accuracy, and is easier to understand. In order to validate the problem, the works of Ma et al. [8] were used and the results were in good agreement related to the present study. The relative error was less than 5%. Therefore, `OpenFOAM` proves to be a proficient and ingenious CFD tool. The use of commercial CFD codes for the analysis of these problems is not a good choice, because of the fact that they are very expensive. Using Open-Source Software (OSS) is an alternative, which is economical for analyzing these problems. The current study involves the investigation of bubble behavior by varying the different transport properties and physical properties. These properties include liquid density surface tension and inlet gas velocity. The variations in bubble diameter, bubble detachment time, bubble agglomeration rates, and liquid surface mixing rates were numerically investigated and different contours and graphs are plotted regarding this matter.

From the investigation, the following conclusions are drawn. With the increment in liquid density, the average bubble diameter, and bubble detachment time reduce considerably but it augments the bubble formation and bubble coalescence frequency. The density variation has a significant impact on free liquid surface mixing rate, i.e., mixing rate increases with increase in bulk liquid density. Surface tension studies show that the bubble diameter and the time of bubble detachment increase with the increment in surface tension, whereas the bubble formation frequency, bubble coalescence rate, and free liquid surface mixing rate shows an inverse proportion relation with surface tension. However, the numerical analysis results indicate that the average bubble diameter increases with increase in inlet gas velocity, whereas the bubble detachment time reduces with the increment in inlet gas velocity. The liquid surface deformation rate increases with increase in inlet gas velocity.

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