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Numerical Analysis of Initial CO_2 Bubbles Leaked in Seawater from Ocean CO_2 Storage using Volume of Fluid Method

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ABSTRACT

The aim of this article is to propose a model to predict initial size and shape of CO_2 bubbles leaked in shallow seawater from ocean CO_2 storage. The volume of fluid (VOF) model in FLUENT was employed. The initial bubble sizes were predicted to increase with the increases in leakage velocity and leakage orifice diameter. The leaked bubbles were predicted to form into various shapes. A comparison of bubble shape predicted by the VOF model and observed from the recently published experimental data showed a reasonable agreement. It was found that the VOF method can be a reliable approach for predicting the initial size and the shape which are used to calculate a rising velocity and a dissolution rate of the bubble during the occurrence of the CO_2 leakage in the ocean.

Keywords: CO_2 leakage; CO_2 bubble; initial size; shape; volume of fluid method.

INTRODUCTION

Deployment of CO_2 sequestrations for mitigating the global warming was believed to be able to reduce CO_2 emissions into the atmosphere to a minimum of 19% in 2050 from which 10% comes from power generation and 9% from industry and transportation [1]. Ocean CO_2 storage is one of the sequestration methods to keep a large amount of CO_2 under the seabed floor [2]. A potential CO_2 leakage from the ocean storage can lead to the environmental impact on marine life due to the ocean acidification between the leaked CO_2 and seawater [3].

Several methods including experiment [4–6] and modelling [7–12] have been conducted to study the leakage behaviour of CO_2 in seawater to detect and to monitor the leak from the shallow ocean storage. In a small field-scale experiment [4, 5] named Quantifying and Monitoring Potential Ecosystem Impacts of Geological Carbon Storage (QICS), 4.2 tons of CO_2 gas were leaked into seawater at depths of 9-12 m at Ardmucknish Bay. The QICS experiment measured pH and pCO_2 (partial pressure of CO_2) of the seawater in a period of 37 days during the occurrence of the leak. It was found that the seawater properties changed in terms of reductions of pH from -1.5 to -2.2 unit and pCO_2 increment of 20-1140 μatm compared with the initial conditions before the CO_2 leaked. The QICS report also noted that the leakage of CO_2 gas in the shallow seawater resulted in a bubble plume which impacted on the quality of the seawater [6]. The findings indicated that the leaked CO_2 bubbles formed in many kinds of shapes with equivalent diameters from 2 mm to 12 mm, with rising velocities in the range of 20-45 cm/s. Some small bubbles were observed to reach the sea surface (0-m depth). In addition, interactions including breakup and coalescence between the CO_2 bubbles have been recorded every second at the first 30-cm height above the sea floor.

An Eulerian-Lagrangian two-phase flow model was applied to simulate dissolution of leaked CO_2 bubbles in the ocean to predict the bubbles behaviour and their termination [7, 8]. Mean initial size of the bubble was set to be 20 mm. Leakage rate was chosen at 6.025×10^{-4} kg/s based on the monitored seepage rate from an existing EOR field. The CO_2 bubbles were simulated to leak from an area of 2 × 10 m at a seabed depth of 200 m. It was demonstrated that all the leaked CO_2 bubbles dissolved in the seawater before spouting up to the atmosphere, and that the increase in pCO_2 in the seawater was smaller than 500 µatm. It was also indicated that the initial size of bubbles had an influence on the dissolution process.

In another modelling method, a two-phase small-scale ocean numerical model was established to simulate the physicochemical behaviour of a CO_2 bubble plume leaked in the North Sea [9, 10]. The initial size of the bubble was calculated between 5 and 8 mm by using Eq. (1). Leakage rates were set to be from 0.1207 to 1 kg/s. The leakage of CO_2 bubble plume was assumed to occur at a 150-m depth of the ocean through a 15-m^2 area. It was found that the leaked bubbles were predicted to fully dissolve in the seawater before reaching the sea surface.

$$\left[(\rho_w-\rho_b)g\frac{d_{eq}^3}{6}\right]^2+\left[\frac{C_d}{8}\rho_w u_{rd}^2 d_{eq}^2\right]^2=\left[d_{ch}\left(\sigma_{b,sed}+\sigma_{w,b}\right)\right]^2 \tag{1}$$

where ρ_w and ρ_b are densities of seawater and CO_2 bubble in kg/m^3, respectively,
g is gravity in m/s^2,
d_{eq} is equivalent diameter of bubbles in m,
C_d is drag coefficient,
u_{rd} is relative velocity of bubble to that of seawater in m/s,
d_{ch} is channel diameter in m,
$\sigma_{b,sed}$ and $\sigma_{w,b}$ are interfacial or surface tensions between bubble/sediment and seawater/bubble in N/m, respectively.

An oceanic two-phase plume model including the calculations of bubble size distribution and bubble interactions (i.e. breakup and coalescence) has been developed to predict the dynamics of rising CO_2 bubble observed from the QICS field experiment [11]. The bubbles were simulated to leak into a computational domain of 50 m length × 50 m width × 9.5 m height with the initial size distribution of 2-12 mm and a 32.1-kg/day leakage rate observed from the QICS project. A total of 35 pockmarks was designed to set the location of the leak. It was found that the model has under-predicted the maximum size of forming bubble and the maximum pCO_2 peak. The simulation predicted the size of 9.8 mm and the partial pressure of 713 µatm, while the observed data from the QICS experiment were at 12 mm and 1500 µatm, respectively. The model also predicted that individual bubbles leaked with the initial size >14mm reach the sea surface and released into the atmosphere.

Currently, an integrated model of the FLUENT-Eulerian model and population balance model (PBM) was employed to simulate the leaked CO_2 bubble plume from the QICS project [12]. This model predicted well the maximum pCO_2 and maximum size of forming bubble. It was found that the predictions from the integrated model are closer to the QICS data compared to the predictions from the oceanic two-phase plume model mentioned above.

The previous modelling methods mentioned above have been applied to predict the leakage behavior of the CO_2 bubbles in various assumptions of initial bubble size. It was found that the initial size of the bubble has strong influence on the dissolution of the leaked CO_2 in the seawater and the release into the atmosphere [11]. Formation of the initial bubble size depends on ocean currents, leakage depths, and channel diameters (e.g. leakage hole) [10]. Effect of these factors on the initial bubble formation was investigated by applying Eq. (1). Shape of the leaked bubble was assumed to be sphere. Thus, the bubble diameters were predicted to decrease with the increase of the depths when there is no ocean currents. It also predicted that the smaller bubble might form with high ocean currents at the 100-m depth. However, this calculation has a limitation on the prediction of the CO_2 bubble shape which consists of small sphere, ellipse and cap [6]. The initial size and shape of the bubbles affect the dissolution rate and the rising velocity [6, 10].

For the study of methane bubble behaviour in a pure water column, the volume of fluid (VOF) model was applied to predict bubble size, shape, rising velocity, breakup and coalescence of the forming bubble [13]. The prediction results of bubble formation and rising had an excellent agreement with the experimental data. The findings indicated that orifice gas velocity and orifice diameter size have the effect on the formation of the methane bubble. The influence of these factors has not yet been experimentally and numerically investigated for the CO_2 bubble formation in the shallow seawater.

This article aimed to simulate the formation of a single CO_2 bubble leaked into shallow seawater for observation of the bubbles behaviour. The VOF model in FLUENT version 17.2 [14] was implemented to numerically analyse the effect of the certain factors (i.e. leakage velocity and leakage orifice) on the initial size and shape of the leaked bubble.

FLUENT-VOF METHOD FOR PREDICTION OF CO_2 BUBBLE FORMATION

Fluent version 17.2 includes the VOF model which can model two or more immiscible fluids by solving sub-models of volume fraction and momentum of the fluids throughout the domain [14]. This model was used to predict initial bubble size, bubble shape, bubble breakup and coalescence as CO_2 bubbles leak into shallow seawater. The description of the sub-models is presented in the following sections.

Volume Fraction Equation

The volume fraction of CO_2 bubble phase in the seawater column is tracked by the solution of a continuity equation, defined in Eq. (2):

$$\frac{1}{\rho_b}\left[\frac{\partial}{\partial t}\left(\alpha_b\rho_b\right)+\nabla\cdot\left(\alpha_b\rho_b\vec{v}\right)\right]=0 \tag{2}$$

where α_b is volume fraction of bubble,

v is velocity of bubble in m/s.

Momentum Equation

The movement of the forming CO_2 bubble and changes in the seawater are tracked by Eq. (3) to (5):

$$\frac{\partial}{\partial t}(\rho\vec{v})+\nabla\cdot(\rho\vec{v}\vec{v})=-\nabla p+\nabla\cdot\left[\mu\left(\nabla\vec{v}+\nabla\vec{v}^{T}\right)\right]+\rho\vec{g}+\vec{F}_{vol} \tag{3}$$

where

$$\rho=\alpha_b\rho_b+(1-\alpha_b)\rho_w \tag{4}$$

$$\mu=\alpha_b\mu_b+(1-\alpha_b)\mu_w \tag{5}$$

where p is pressure in Pa, and μ is viscosity in Pa.s.

Continuum Surface Force Model

Equation (6) describes the conversion of surface tension into a body force acting on the interface. This force is added to the calculation of the momentum equation mentioned above.

$$F_{vol}=\sigma_{w,b}\frac{\rho\kappa_b\nabla\alpha_b}{\frac{1}{2}(\rho_b+\rho_w)} \tag{6}$$

where:

$$\kappa_b=\nabla\cdot\hat{n} \tag{7}$$

$$\hat{n}=\frac{n}{|n|},\ n=\nabla\alpha_b \tag{8}$$

where κ is curvature, n is surface normal

CASE STUDIES AND COMPUTATION APPROACH

Case Studies

The initial CO_2 bubble was assumed to form after leaking through a small orifice into a stable seawater column. Some case scenarios were conducted to sensitively investigate the effect of leakage velocity and orifice diameter size on the bubble formation, and are listed in Table 1. The orifice sizes were chosen based on Dewar et al.'s study [10]. The leakage velocities were considered as the rising velocity of the leaked bubble observed from the QICS experiment [6]. Table 2 shows the physical properties of the CO_2 and the seawater measured at 10 °C for all case scenarios.

Table 1. Setting values of case studies.

Case	Orifice size (mm)	Leakage velocity (m/s)
1	4	0.15
2	4	0.25
3	4	0.35
4	6	0.25
5	8	0.25

Table 2. Physical properties of CO_2 and seawater used to set material properties in the simulation.

Properties	Unit	CO_2	Seawater
Viscosity	Pa.s	14.2×10^{-3}	1.4×10^{-3}
Density	Kg/m3	1.9	1027
Surface tension	N/m		7.37×10^{-2}

Computation Approach

The Design Modeller in Ansys Workbench version 17.2 was applied to generate a computational domain with 1 m in Y-axis and 0.076 m in X-axis to simulate the CO_2 bubble formation in the seawater. A total of the five cases were presented as in Table 1 to allow the CO_2 leak into the domain through a small orifice with different diameter sizes. The inlet and outlet boundary conditions were defined as velocity inlet and pressure outlet, respectively. All the walls were considered to obtain no-slip boundary condition. The operating pressure was set at 101,325 Pa at a point of X = 0.038 m and Y = 1 m. The solution method was chosen based on the previous study by Pourtousi et al. [13]. Thus, the quadric upwind interpolation (QUICK) method was used to numerically solve the governing equations. The velocity and pressure were coupled using the PISO (pressure implicit split operators). The under-relaxation factors of 0.3 and 0.7 were taken for pressure and momentum, respectively. The formation of the bubble was simulated by employing the transient model with a time step of 0.0001s and the Courant number of 0.25.

RESULTS AND DISCUSSION

Grid dependency

The domain generated above was divided into several discrete cells using the Meshing software in Ansys Workbench 17.2. Quadrilateral grids were used for this grid generation. To test the impact of computational domain and grid size, three different grids were conducted to ensure the independence of solution from the domain and the grid size as shown in Table 3. Figure 1 presents the surface grids of the computational domain with 304,000 cells.

The study of grid dependency was tested on the distance of the first bubble after been formed and its rising velocity with different time as illustrated in Figure 2. It was found that there is a small difference in the prediction results from the current and finer grids. Thus, the current grid was considered for the rest of the case scenarios due to computational cost and accuracy.

Model validation study

As mentioned earlier, there is lack of experimental data on the formation of initial CO_2 bubble size in the seawater. Hence, the validation study was carried out by comparing the initial bubble size predicted from the VOF model and from a mathematical model in Eq. (1); used in the study of Dewar et al., (2013b). The equation (1) cannot account for effects of pressure on the initial bubble formation. The pressure can cause the bubbles to be forced out of the leakage hole and the bubbles can merge to become a bigger bubble [10]. Figure 3 shows the comparisons of the initial size predicted by the VOF model and the mathematical model. It indicated that the VOF model is consistent with the mathematical model.

In another model validation study, a comparison of the bubble shapes after detachment, coalescence, and breakup predicted from the VOF model and observed from the QICS experiment [6] is carried out and is illustrated in Figure 4. It was found that there is a reasonable agreement between the simulation and the published experimental data.

Table 3. Grids conducted for dependency study.

Grid type	Element size (mm)	Number of cells
Finer	0.4×0.4	473,480
Current	0.5×0.5	304,000
Coarser	0.8×0.8	118,465

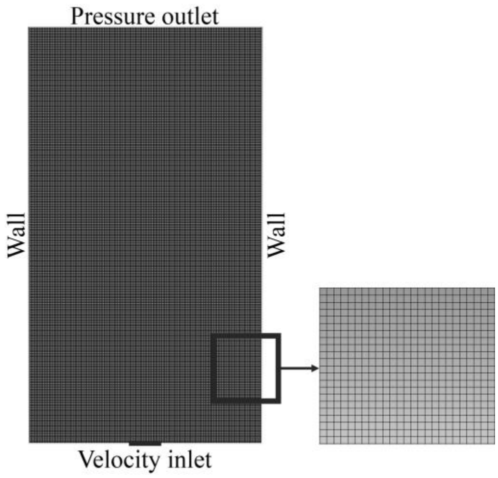

Figure 1. A surface grid of domain with 304,000 cells and boundary conditions.

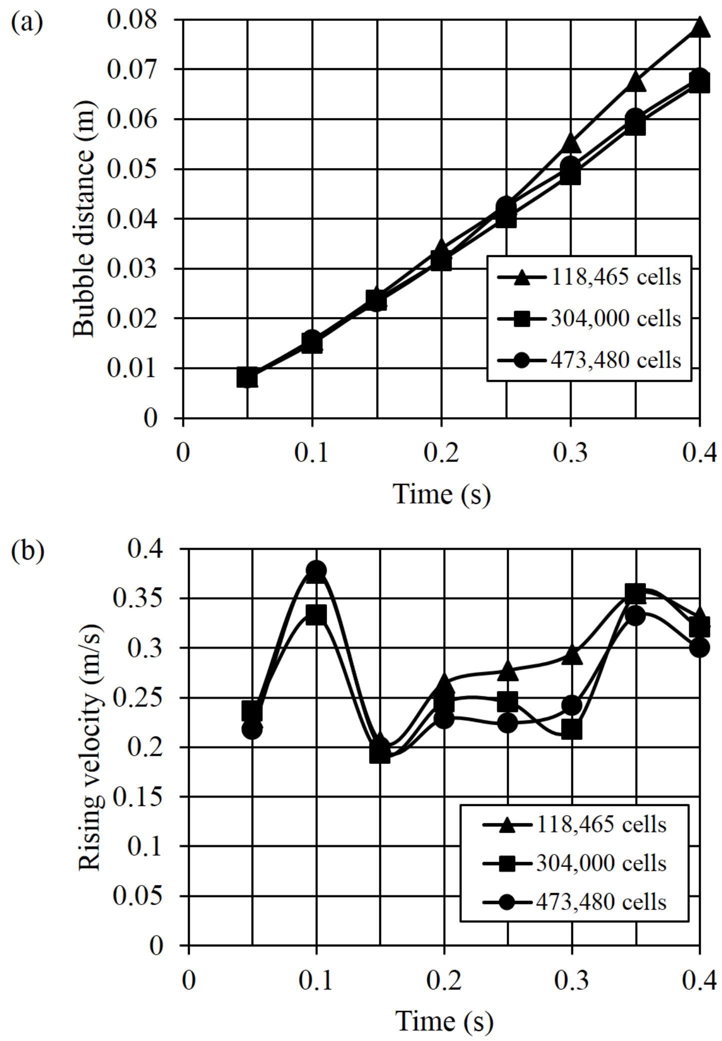

Figure 2. Grid dependency was studied with three different grids on (a) bubble distance measured from the leakage hole and; (b) rising velocity of formed bubbles.

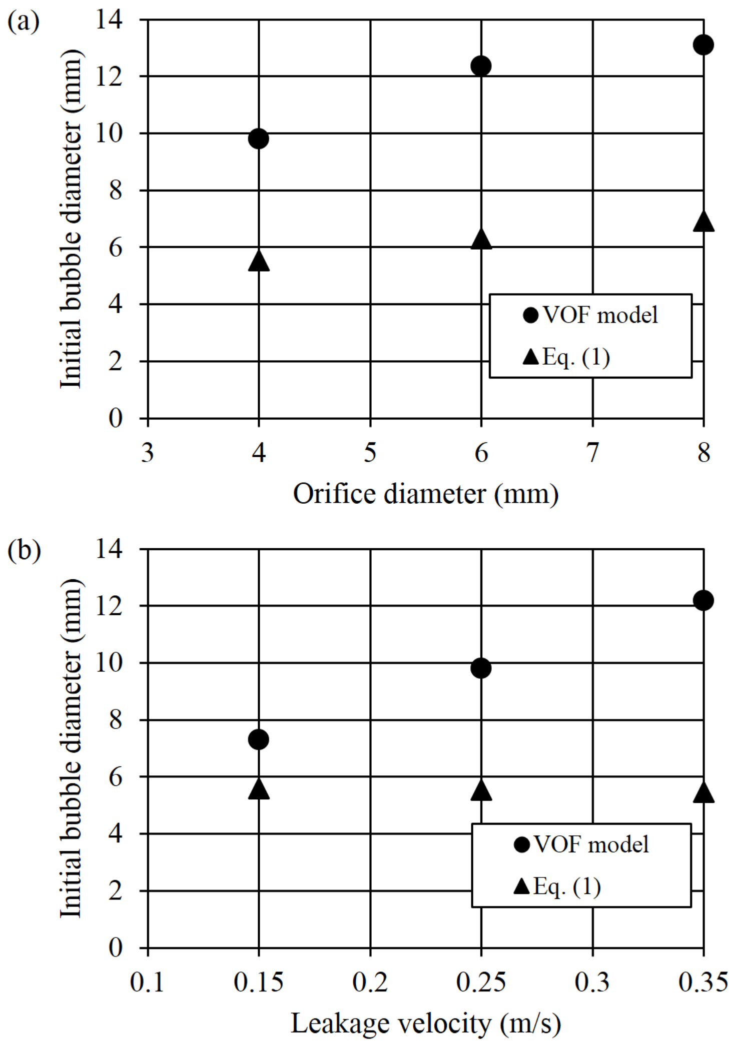

Figure 3. Comparison of initial CO_2 bubble size predicted by VOF model and Eq. (1) at (a) 0.25 m/s leakage velocity and; (b) 4 mm diameter of the orifice with different leakage velocities.

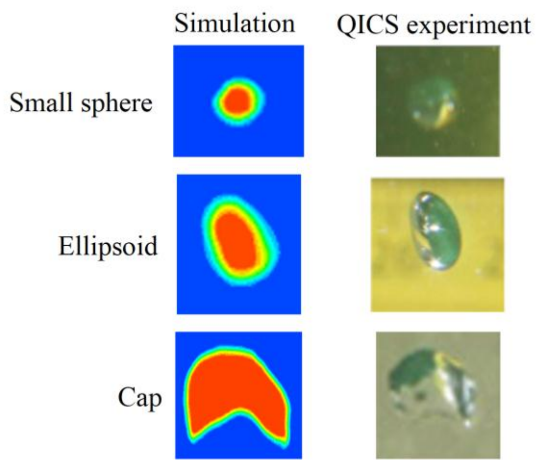

Figure 4. Comparison of bubble shapes.

Analysis Results and Discussion on the CO_2 Bubble Formation

Figure 5 shows the simulation results of the CO_2 bubble formation for case 1, 2 and 3. The leakage velocity was set at 0.15, 0.25 and 0.35 m/s, respectively. A 4-mm diameter leakage orifice was used to simulate for all these case scenarios. It can be noted that a larger initial bubble size is predicted to form for the case with higher leakage velocity. The first bubble formed in the case with higher leakage velocity is predicted to coalesce with the second bubble at a faster time compared to the cases with lower gas velocity. It was also simulated that the breakup of the third bubble in the case 3 occurs faster than the cases 1 and 2.

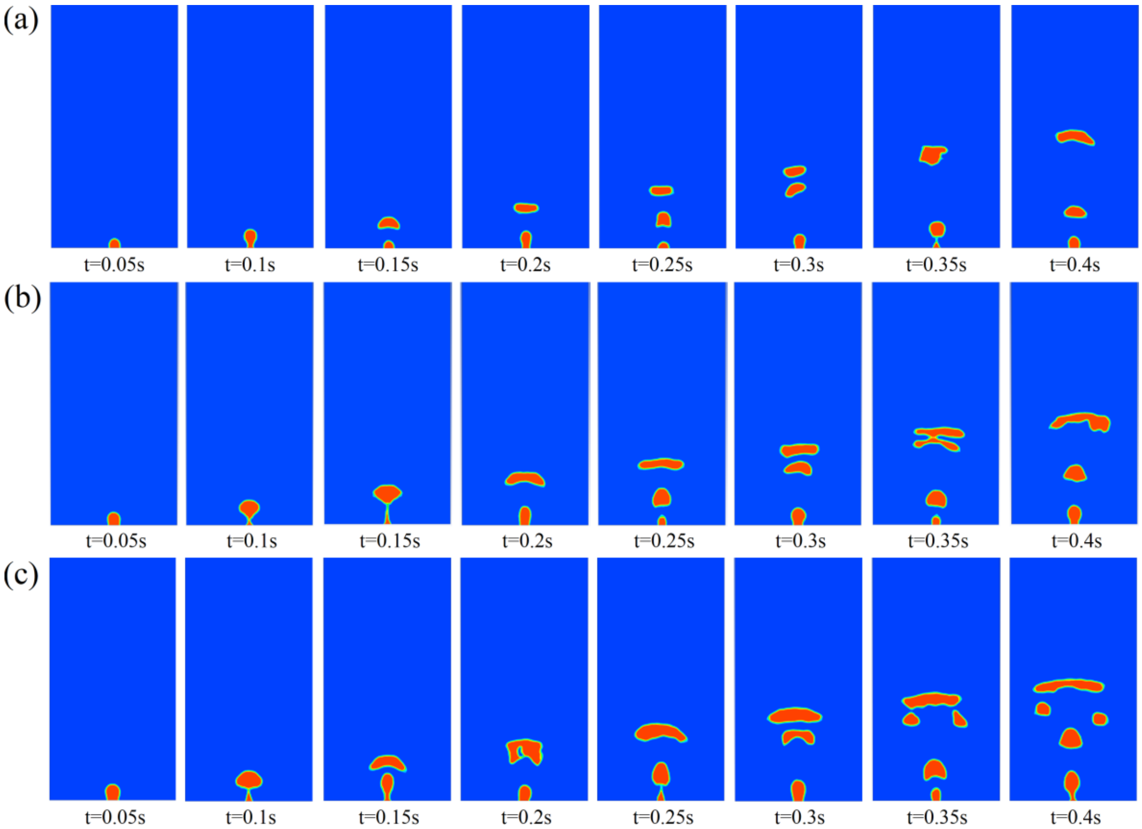

Figure 5. Predictions of bubble formation after leaking through a leakage hole of 4-mm diameter for (a) case 1, (b) case 2 and; (c) case 3.

The cases 2, 4 and 5 were designed to numerically study the impact of leakage orifice on the formation of CO_2 bubble in the seawater, as presented in Figure 6. A 0.25-m/s leakage velocity was set to allow the CO_2 gas leak through three various orifice sizes from 4 mm to 8 mm. It was predicted that the initial bubble size increases as the diameter of the orifice increases. For the case 5, the coalescence of the first and second bubbles, and the breakup of the third bubble were predicted to occur faster than the cases 2 and 4.

For the case of CO_2 leakage in seawater, the larger bubbles are formed at higher velocity, hence it will rise faster. While smaller bubbles have more interfacial area at a certain leakage velocity, so it will fully dissolve quicker [6, 10]. It can be observed in Figures 5 and 6 that the bigger bubble rises faster than the smaller bubble for all the simulation cases. It was also predicted that the leakage cases with the higher leakage velocity and the larger orifice size produces a larger amount of smaller bubbles. This can cause the increase in the dissolution rate of the leaked CO_2.

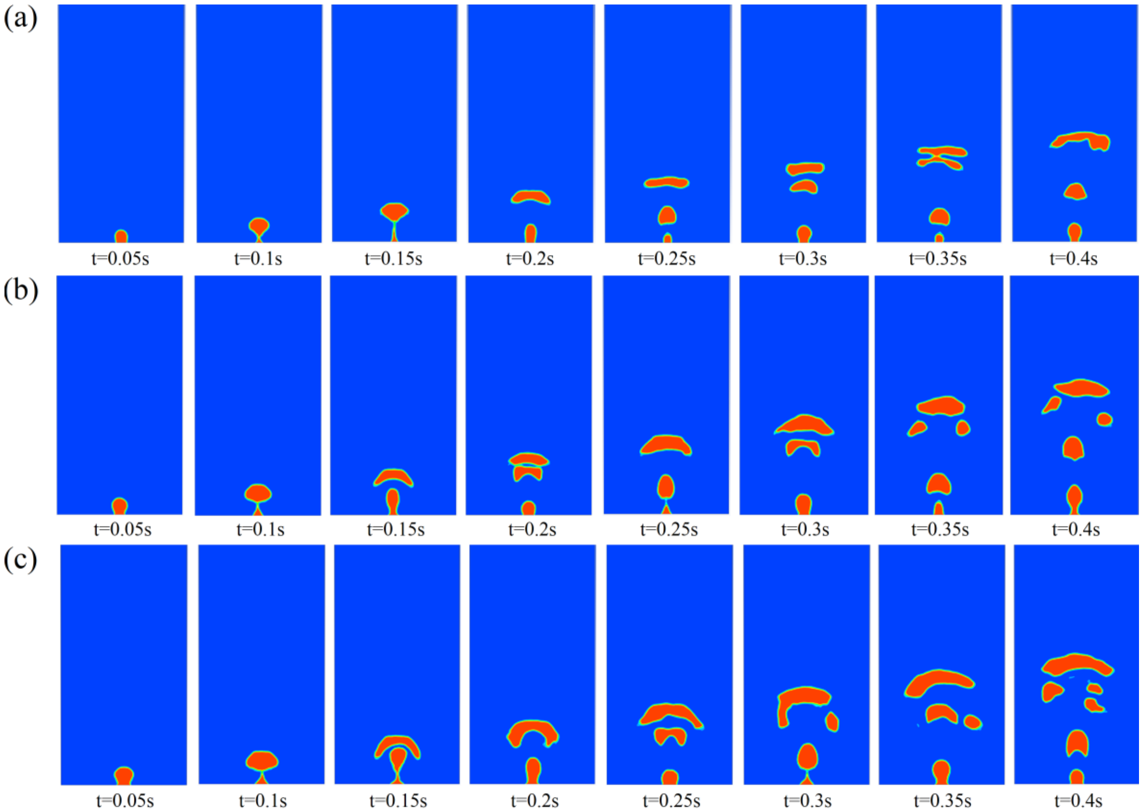

Figure 6. Predictions of bubble formation after leaking with a constant of 0.25 m/s leakage velocity for (a) case 2, (b) case 4 and; (c) case 5.

CONCLUSION

In this study, the VOF model was employed to numerically study the formation of CO_2 bubbles in the seawater. This method can calculate the initial size and the shape which determine the rising velocity and the dissolution rate of the bubble in the leakage event of the ocean CO_2 storage.

Five case scenarios were designed to simulate the impact of the leakage velocity and size on the bubble size. The bigger bubble is produced by increasing the leakage velocity. This is due to higher bubble velocity and coalescence. As the leakage size increases, the bubble wake will be stronger due to the larger bubble size. Subsequently, the bubble size will be bigger and the rising velocity will be changed.

The shape of the bubble after detachment, coalescence and breakup was predicted to change into various shapes of sphere, ellipsoid, and cap. It was found that the bubble shapes predicted from the VOF model and observed from the QICS experiment had a reasonable agreement.

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