Rising Characteristics of a Methane Bubble under Different Conditions: A CFD Study

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Abstract. For a methane (CH₄) bubble rising in liquid, knowledge of bubble rising characteristics is crucial for the comprehension of methane dissolution rate and the inter-phase mass transfer. Here, the investigation of a methane bubble was performed using the computational fluid dynamics (CFD) technique and the volume of fluid (VOF) two-phase model. The deionized water of 13 MPa and 5°C was used as the carrier of the rising bubble. Bubbles with diameters ranging from 3.0–6.0 mm were selected. The results show that the bubble instantaneous liquid velocity distribution and the wake structure manifest unique characteristics under such a high-pressure and low-temperature condition. The bubbly flow involves complicated vortex structures. Moreover, the bubble velocity is relatively low relative to those obtained under general conditions. A non-dimensional analysis of the bubble behavior indicates that the results obtained here deviate significantly from available results obtained under general conditions. The bubble diameter significantly influences the drag coefficient.

1. Introduction
Methane (CH₄) seepage in liquid mediums from natural vents and industrial pipelines has been an alarming phenomenon reported globally. As CH₄ gas hydrate is produced in water bodies, it becomes an important source of energy. However, it often has the propensity to ascend unless it is completely dissolved in the liquid. During the dissolution process, the CH₄ hydrate (which cages the CH₄ gas bubbles during formation at high-pressure and low-temperature) is anaerobically oxidized by a conglomerate of CH₄-oxidizing microorganisms, forming a filter to trip dissolved CH₄ from entering the water body. The difficulty of efficiently detecting the rising CH₄ bubble in liquid mediums is apparent.

Characteristics of CH₄ bubbles under high pressure and low-temperature conditions have received tremendous attention over the past decades. Many researchers have obtained datasets by releasing, tracking and filming CH₄ bubbles in clean water (reservoirs, lakes, rivers) and contaminated water (continental shelves, continental slopes, oceans) to develop correlations between the two phases [1, 2]. Heretofore, experimental results under such conditions have scarcely been reported hence giving rise to the need to explore computational techniques.

The computational fluid dynamics (CFD) technique assumes an important role in describing characteristics of bubbly flows, particularly under harsh conditions. The volume of fluid (VOF) two-phase model has the advantages of easy realization, low computational complexity, and high precision. Numerical studies on bubbles in both Newtonian and non-Newtonian fluids have been performed using the VOF model [3, 4]. The rising characteristics of a bubble are largely influenced by its size, rising
trajectory, and properties of the surrounding liquid. During the rising process, small bubbles retain a spherical shape while large bubbles are prone to rapid deformation and velocity fluctuations. However, further work is still needed in the quantitative characterization of the bubble velocity fluctuations and the prediction of the hydrodynamic forces acting on it.

The motivation of the present study is drawn from the reported cases of the rapid seepage of CH$_4$ gases from natural sources, including contaminated and noncontaminated regimes, and thermogenic sources, including pipeline leakages and accidents occurring in oil and gas production [5]. Furthermore, a substantial understanding of bubble behavior under extreme conditions is crucial for unlocking deeper insight into relevant applications. In the present study, the CFD technique and the VOF model were used to simulate the motion of CH$_4$ bubbles in deionized water (DI-H$_2$O) at 13 MPa and 5 °C. The bubble diameters ranged from 3.0 to 6.0 mm.

2. Governing Equations and Two-phase Model
The volume of fluid (VOF) method was used to track the volume fraction (F) of each phase to determine the phase and interface of the computational domain. In the VOF model, a single continuity and momentum equations were solved throughout the domain. The Continuum surface force (CSF) model and the piecewise linear interface calculator (PLIC) were adopted to compute surface tension and interface reconstruction, respectively. A computational domain of 100×180 mm was constructed. The grid number of 375,298 was considered reliable and adopted for the simulation. Initially, a single bubble was inserted into the computational domain with the symmetry center of the bubble at (x=0, y=20.0 mm). Properties of the two phases at 13 MPa and 5°C were listed in Table 1. Three bubble diameters, D$_b$, of 3.0, 4.5 and 6.0 mm would be covered in the simulation. The commercial CFD software ANSYS FLUENT served as the solver.

| Phase   | Density /kg·m$^{-3}$ | Surface tension /N·m$^{-1}$ | Dynamic viscosity /($\times$10$^{-3}$)Pa·s |
|---------|----------------------|----------------------------|------------------------------------------|
| DI-H$_2$O | 1006.2               | 0.0531                     | 1.4982                                   |
| CH$_4$  | 117.56               |                            | 0.015628                                 |

Table 1. Physical properties of the two phases

Fig. 1 Bubble rising velocity per time for air bubble in water, data from [6, 7] are included.

3. Validation of the Numerical Scheme
The numerical scheme was validated through a comparison between the simulated results and the results reported in [6, 7] where the air bubble of D$_b$=4.0 mm was studied. As shown in Fig. 1, variations of the bubble rising velocity with the bubble rising time were plotted. The rising velocity in the first 0.05 s is relatively high for the current result and the results obtained by Ma et al. [6]. The overall result obtained here is quite consistent with those published, as indicated in Fig. 1.
4. Results and Discussion

4.1. Bubble Trajectory

The rising characteristics of a single CH₄ bubble in deionized water at 13 MPa and 5 °C are analyzed at a time interval of 0.04 s between adjacent bubbles. For all cases, the bubbles start from rest, ascend in a disk-like shape and then either maintain rectilinear trajectory or adopt a wobbly path with bubble deformation.

As can be seen in Fig. 2, bubbles with different sizes exhibit different rising behaviors. In Fig. 2(a), the bubble initially starts from rest, adopts and maintains a rectilinear path for $t=27.25s$ at $y=64$ mm and then, retains zigzagging for the subsequent journey. At $D_b=4.5$ mm, the bubble adopts and maintains a rectilinear path throughout its journey, as shown in Fig. 2(b). The trajectory of $D_b=6.0$ mm is similar to that of $D_b=4.5$ mm, as seen in Fig. 2(c). However, the bubble exhibits relatively complicated shape and manifest remarkable deformations.

![Fig. 2](image_url)

**Fig. 2** Single bubble rising trajectories at a time interval of 0.04 s between adjacent bubbles for (a) $D_b=3.0$ mm; (b) $D_b=4.5$ mm; (c) $D_b=6.0$ mm

4.2. Instantaneous Velocity and Wake Characteristics

In Fig. 3, the velocity distributions and wake characteristics of bubble rising in deionized water of 13 MPa and 5 °C at 46 mm were investigated as presented. The bubble initially starts from rest and rises due to buoyancy, forming a liquid jet in its wake. The jet pushes the bubble’s lower surface towards its upper surface, causing pressure fluctuations. These fluctuations lead to the formation of vortices. Different bubble diameters and mediums result in completely different vortex patterns, however; their initial rising stages are accompanied by rectilinear trajectories which are antecedents of stable bubbles wake. For all cases, the bubble initially starts in a rectilinear path, which is associated with vortices and recirculation zones. As the bubble progresses upward, it changes horizontal positions as the vortices become vivid, as indicated in Fig. 3(a). For $D_b=4.5–6.0$ mm, relatively more complex coexisting vortices arise as the bubbles become exposed to greater deformations, overlying resistances and shape transformations influenced by wake shedding. The accumulation of unequal vortices in the bubble wake leads to the evolution of recirculating rings which contribute to the bubble shape transformation, as can be been in Fig. 3(b) and (c).

Consequently, the overall vortex structure under such conditions is complicated relative to normal conditions. Moreover, the bubble size is a major parameter in determining the bubble vortex structure as larger bubbles are associated with more complex vortices, as well as velocity distributions.
Fig. 3 Velocity distributions surrounding the bubble at y= 46.0 mm: (a) Db=3.0 mm, ts= 0.1725 s; (b) Db=4.5 mm, ts= 0.185 s; (c) Db=6.0 mm, ts= 0.20 s.

4.3. Variation of Bubble Velocity
Here, the centroid coordinate (x,y), as well as the major and minor axis, is used to calculate the bubble displacement and then, the bubble velocity at a given displacement is computed. The variation of bubble velocity with the displacement is illustrated in Fig. 4(a) for various bubble sizes. Initially, the bubble starts from rest, accelerates and decelerates, causing velocity fluctuations as it rises. Hence, the average terminal velocity of the bubble is calculated right after the bubble reaches its terminal velocity and is considered as the main local velocity, as presented in Fig. 4(b). A direct assessment of the terminal velocity is defined as [9]:

\[ V_T = \sqrt{\frac{2\sigma}{d \rho l} + \frac{8d \rho g}{\rho l^2}} \]  

The calculated velocity is approximately 0.2 m/s while the simulation result of the bubble velocity is not stable but fluctuates between 0.10 and 0.24 m/s. The mean local velocities for D_b of 3.0, 4.5 and 6.0 mm are approximately 0.17, 0.16 and 0.15 m/s respectively. The bubble velocity is relatively low due to the influence of low temperature and high-pressure conductions.

Fig. 4 Variation of bubble velocity as the bubble rises

4.4. Non-dimensional Analysis
To quantitively explicate the bubble shape evolution, a comparison of the bubble aspect ratio, E, with respect to y is illustrated in Fig. 5. The bubble exhibits different shapes during its rising process. Initially, E starts from a stable state (E=1.0) but begins to fluctuate as the bubble adopts a wobbly path. The shape and range of E evidently differ for each bubble size and evolve with respect to time and displacement, as illustrated in Fig. 5(a) and (b).
As the bubble rises upward, the primary forces exerted on the bubble are the drag force and the buoyant force. The drag force presumes an important role in elucidating the bubble hydrodynamics. As the bubble rises at a constant velocity in a quiescent liquid, the balance between the drag and buoyancy forces is given as:

$$C_D \frac{1}{2} \rho_i V_T^2 \frac{\pi d_e^2}{4} = (\rho_i - \rho_g) g \frac{\pi d_e^3}{6}$$ \hspace{1cm} (2)

where $C_D$ is the Drag coefficient. In the initial stage, the bubble starts from rest and the drag force is zero. The difference in the fluid density and gravity causes the bubble to rise. As the bubble accelerates during the bubble rising process, the drag force on the bubble increases subsequently, leading to a reduction in acceleration. This process continues until the bubble terminal velocity is reached where the buoyancy, drag and gravity forces are balanced. In the present study, $C_D$ is investigated and compared with the correlation from Batchelor et al. [10]:

$$C_D = \frac{4(\rho_i - \rho_0)g d_e}{3 \rho_i V_T^2}$$ \hspace{1cm} (3)

The measured and calculated $C_D$ are plotted in Fig. 6. In comparison, the drag coefficients obtained using the empirical formula are small and are featured by nearly equivalent values as Re varies. For the results obtained here and under high pressure and low-temperature condition, the overall drag coefficient is considerably high. Meanwhile, the smallest bubble diameter is responsible for low Re and drag

**Fig. 5** Variation of bubble aspect ratio with $y$ and $t$

**Fig. 6** Variation of CD with Re for different bubble sizes
coefficients. At $D_b=4.5$ mm and 6.0 mm, although the data points are scattered, the drag coefficient magnitudes are similar and the Re associated with $D_b=6.0$ mm is slightly high.

5. Conclusion

(1) Rising characteristics of the bubble under the conditions considered are complicated relative to normal conditions. Bubbles with diameters of 4.5 and 6.0 mm exhibit coexisting vortices.

(2) The local mean velocity, calculated after the bubble reaches its terminal point, agrees with the theoretical correlation by Mendelson et al. The overall terminal velocity is relatively low due to the influence of operating parameters.

(3) The non-dimensional analysis of the bubble behavior indicates that the results obtained under high pressure and low-temperature condition deviate significantly from the results obtained under normal conditions. The bubble diameter influences remarkably the drag coefficient.

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