Numerical simulation of the motion of a free rising air bubble

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Abstract. In this work the results of numerical simulation of the motion of a free rising air bubble in the water are presented. The calculations were performed for bubbles with different diameters in the range from 1 to 10 mm. Calculated parameters of the trajectory and the average rising velocity were compared with the experimental data. The vortex flow behind the bubble was analyzed. Multidirectional circulations were found. The imbalance between these circulations causes the vertical deviation in the trajectory.

1. Introduction
Today, the process of bubble’s rising is not well studied and described, it is caused by a variety of physical phenomena in this problem and significant size differences. Experimental study of this problem requires the use of modern, high-precision detection tools [1, 2] and the numerical simulation is impossible without large computational resources [4, 5].

Small-size bubbles have great importance at the industry. Bubble flows can be observed in the various industrial processes: bubble column, intermixing reactor, flotation, sedimentation. Cavitation is the main rupture source for pipelines and screw propellers. All these processes depend on the concentration, sizes and rising velocities of the bubbles.

2. Physical model and numerical method

2.1. Governing equations
To simulate the rising bubble in water, we assumed that the rising occurs in an incompressible viscous liquid at a constant temperature. The movement of the liquid around the bubble is described by the solution of the equation of continuity, Navier-Stokes equations and the continuity equation for the volume concentration of water:

\[ \nabla \vec{U} = 0 \]  

\[ \frac{\partial}{\partial t}(\rho \vec{U}) + \nabla (\rho \vec{U} \times \vec{U}) = -\nabla P + \nabla (\bar{\tau}) + \rho g + \vec{F}_{vol} \]  

\[ \frac{\partial}{\partial t}(c_i \rho_i) + \nabla \cdot (c_i \rho_i \vec{U}) = 0 \]

where \( \rho \) – density, \( \vec{U} \) – velocity, \( P \) – pressure, \( \bar{\tau} = \mu (\nabla \vec{U} + \nabla \vec{U}^T) \) – viscous stress tensor, \( \mu \) – dynamic viscosity, \( g \) – acceleration of gravity, \( \vec{F}_{vol} \) – exterior volume force, \( \rho_i \) – density of \( i \)-th phase, \( c_i \) –
concentration of \( i \)th phase. The air concentration in each control volume was calculated based on the normalization condition per unit:
\[
\rho = \rho_i c_i + \rho_j (1 - c_j).
\]
The action of surface tension forces is described by the value of continuous volume force:
\[
\tilde{F}_{\text{vol}} = \sigma \rho h \nabla c_{\text{Air}} (0.5(\rho_{\text{Air},0} + \rho_{\text{Air}}))^{-1},
\]
where \( \sigma \) – surface tension coefficient, \( \kappa = \nabla \cdot \hat{n} \) – surface curvature, \( \hat{n} = \hat{n} / |\hat{n}| \) – unit surface normal. This method is called Continuum Surface Force Model (CSF) [6].

The SIMPLE method was used to solve the Navier-Stokes equations. To calculate the motion of a multiphase liquid and determine the phase interface, the VOF method was used [7]. When calculating the flow of two-phase liquids there is a problem of blurring the phase boundary due to the diffusion of one liquid to another. To reduce this effect, different techniques are used. For example, in [8] and [9], special terms are added to the continuity equation for the volume concentration of the phase (3). These terms act on the interface and reduce the diffusion of one phase to another. Therefore, equation (3) takes the following form:
\[
\frac{\partial c}{\partial t} + \nabla (c \tilde{U}) + \nabla [c(1-c)\tilde{U}] = 0
\]
where \( c \) – concentration of first phase, \( \tilde{U} = f(\nabla \alpha) \) – compressive velocity. Compaction of the liquid-gas interface is determined by the multiplier \( c(1-c) \), which has a maximum value at the phase boundary (0.25) and tends to zero when \( c \) tends to 0 or 1 [8].

Figure 1 illustrates the schematic diagram of the numerical simulation, where \( d_b \) – bubble diameter, \( h \) – height of bubble initialization, \( H \) – mesh height, \( L \) – base width, \( \rho_1, \mu_1 \) – air parameters, \( \rho_2, \mu_2 \) – water parameters.

The sizes were chosen with the view of minimizing the influence of boundaries on the dynamics of bubble’s rising and minimizing the size of the grid. The boundary conditions were set as follows: on the side boundaries – the symmetry condition, on the upper boundary – the velocity inlet condition, on the lower boundary – the free outflow condition.

**Figure 1.** Schematic diagram of the numerical simulation.

In all simulations were used the following material properties: \( \rho_1 = 1.225 \) kg/m\(^3\), \( \mu_1 = 1.789 \cdot 10^{-2} \) mPa·s, \( \rho_2 = 998.2 \) kg/m\(^3\), \( \mu_2 = 1.003 \) mPa·s, \( \sigma = 0.072 \) N/m.

2.2. Moving frame
When modeling the bubble’s rising to a height of more than 10 cm, it is necessary to use grids with the number of cells about 10 million. To reduce the mesh, a moving frame approach was used. Let XYZ is a fixed coordinate system, \( X'Y'Z' \) – a moving coordinate system, \( U \) – the velocity in a fixed coordinate system, \( U' \) – the velocity in a moving coordinate system, and \( U_m \) – the velocity of a moving coordinate system, then:
\[ \dot{U}(x, y, z, t) = \dot{U}'(x', y', z', t) + \dot{U}_m(t) \quad (6) \]

Since the X'Y'Z' coordinate system is noninertial, the equation (2) takes the form:

\[ \frac{\partial}{\partial t} (\rho \dot{U}') + \nabla (\rho \dot{U}') = -\nabla P + \nabla (\rho \ddot{z}) + \rho \ddot{g} + F_{vol} - \rho \frac{d}{dt} \dot{U}_m(t) \quad (7) \]

The value \( U_m(t) \) was calculated as the velocity of the bubble center of mass in the X'Y'Z' coordinate system, and was used as a flow boundary condition with a reverse sign. As a result, the velocity in the fixed coordinate system, calculated by the formula (7), was close to zero, and the bubble actually rested. The use of a moving coordinate system significantly increased the accuracy and reduced the calculation time. This approach allowed carrying out calculations for bubbles with diameters of 1 and 2 mm in a reasonable time.

3. Numerical results

3.1. Parameters of the trajectory

Figure 2 shows the bubble center of mass trajectories for different diameters in the XYT coordinate system. It can be seen that for bubbles with diameters of 3; 4 and 5 mm there is a stable spiral motion. The bubbles with diameters of 2 and 6 mm have a combined trajectory: a zigzag mode at the initial part of the rising that switches to a stable spiral mode. For a 10 mm bubble, the trajectory looks like a spiral. For a 1 mm diameter bubble, the trajectory is close to the vertical, so its trajectory is not shown in figures 2 and 3.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{bubble_trajectories.png}
\caption{The paths of the bubbles in XYT: (a) \( d_b = 2 \) mm, (b) \( d_b = 3 \) mm, (c) \( d_b = 4 \) mm, (d) \( d_b = 5 \) mm, (e) \( d_b = 6 \) mm, (f) \( d_b = 10 \) mm.}
\end{figure}
The projections of the bubble’s paths on the planes XZ, YZ was obtained. Comparison of the dependences X(t) and Y(t) shows the oscillation dynamics (figure 3).

Figure 3. The dependences X(t) and Y(t): (a) \(d_b = 2\) mm, (b) \(d_b = 3\) mm, (c) \(d_b = 4\) mm, (d) \(d_b = 5\) mm, (e) \(d_b = 6\) mm, (f) \(d_b = 10\) mm.

Table 1 presents the calculated values of the average amplitude \((\bar{X}_{\text{max}}, \bar{Y}_{\text{max}})\) and the period of the bubble’s oscillations. The value \(A\), which is presented in the table is defined as: \(A = \sqrt{\bar{X}_{\text{max}}^2 + \bar{Y}_{\text{max}}^2}\). Analyzing the dependences X(t) and Y(t) for the bubble with diameter of 3 mm presented in [2], it was concluded that the amplitude and the period of oscillations in the experiments are greater due to the imperfect purity of water and air.

Table 1. Parameters of the trajectory for various bubble diameters.

| \(d_b\) (mm) | \(\bar{X}_{\text{max}}\) (mm) | \(\bar{Y}_{\text{max}}\) (mm) | \(A\) (mm) | \(T\) (sec) | Path form               |
|-------------|----------------|----------------|--------|--------|-------------------|
| 2.0         | 1.0            | 0.5            | 1.1    | 0.05   | Zigzag and helical motion |
| 3.0         | 2.0            | 1.5            | 2.0    | 0.08   | Helical motion    |
| 4.0         | 2.5            | 1.8            | 3.1    | 0.09   | Helical motion    |
| 5.0         | 1.75           | 1.75           | 2.5    | 0.10   | Helical motion    |
| 6.0         | 1.65           | 1.65           | 2.3    | 0.12   | Zigzag and helical motion |
| 10.0        | 1.43           | 1.41           | 2.0    | 0.16   | Helical motion    |

3.2. The average rising speed

Figure 4 shows a comparison of the calculated values of the average bubble rising speed \((U_b)\) with experimental data [1,2]. For both areas of experimental data (blue and red curves), the upper curve corresponds to pure water experiments, the lower curve corresponds to experiments with contaminated water. The calculated values of \(U_b\) lie within the range of the experimental data. In the calculations, there are no bifurcations of the speed obtained experimentally. Traditionally this bifurcation has been explained by the presence of surfactants (contaminated water) or by the variations of forms of the initial bubbles (sphere or ellipsoid). In the calculations carried out, the bubble during initialization is an ideal sphere, and impurities in the water are not modeled. Reproduction of bifurcation in the calculations will be very important to explain the experiments. The table in the right of the figure 4
shows the average values of $U_b$ for different bubble’s diameters. The good agreement of numerical calculation with experiment for all range of calculated values is seen. The value of the Z- component of the velocity of the bubble center of mass for a bubble of arbitrary diameter increases rapidly at first, and then fluctuates near a constant value. In the article [2] the average bubble rising speed ($d_b = 3$ mm) of the order of $\sim 20$ cm/s, which is in good agreement with the calculated value (see figure 4). The period of oscillation of $U_z$ in the experiments: $0.08–0.10$ s; in the results of calculations: $\sim0.06$ s.

Figure 4. Comparison calculated values of $U_b$ with experimental data.

4. Analysis of vortex flow behind the bubble
For the analysis of vortex flow behind the bubble was considered a three-dimensional field of Z-components of vorticity in the wake of the rising bubble. Figure 5(a) shows the formation of "vortex tails" rotating around the bubble’s trajectory. The scale of "vortex tails" grows after the beginning of the rising.

Figure 5(b) shows a graph of change of the circulation velocity behind the bubble for different horizontal cross sections (shift from the bubble bottom is 2.0–3.2 mm) depending on the radius of the contour $R$. The contours with $R$ of 0.5 to 6.0 mm were considered. The graph shows that one direction of the rotation is dominant and that the tail with the opposite direction with the growth of the distance to the bubble becoming inside the more powerful tail. These multidirectional circulations of the velocity in the horizontal plane generate the imbalance in flow around and behind the bubble and cause the vertical deviation in the trajectory.
5. Numerical data postprocessor
In the course of the calculations there was a problem of processing huge amounts of data (data size of the one calculation is about 100 Gb). Initially, the data storage format was replaced by the binary format CGNS (CFD General Notation System). But the time of manual processing for one calculation was several hours as before. Therefore own program for post-processing of results was created. Using the postprocessor has reduced the time of data processing to 10 min. All data processing algorithms are written in C++ programming language with Qt Framework. The graphical shell (GUI) is created in Qt Designer. The program provides a wide functionality for post-processing of calculation results and can be quickly adapted to other tasks. The program allows obtaining trajectories, shapes and vortex traces for rising bubbles. All graphs and fields of values presented in this article are obtained using this postprocessor.

6. Numerical results
The work on numerical simulation of the motion of a free rising air bubble with different diameters is carried out. It is shown that bubble’s trajectory is a stable spiral or a combined trajectory: a zigzag mode at the initial part of the rising that switches to a stable spiral mode. The period and amplitude of the trajectories for all simulated bubble sizes are calculated and the average rising velocity is calculated. The obtained values are consistent with experimental data [1,2]. However, the amplitude and the period of oscillations in the experiments is greater than in CFD calculations due to foreign substances in real water and air.

Calculations have shown that the period of oscillations increases with the diameter of the bubble, while the amplitude of oscillations with the diameter increases first and after it reaches a maximum then falls. This behavior of the amplitude is due to the fact that with the increase of the diameter bubbles becoming more flattened and the increased drag force stabilizes the rising and not allows the bubble to deviate from the vertical stronger. The initiation of multidirectional circulations of the velocity in the horizontal plane behind the bubble was shown. It is assumed that the imbalance between these circulations causes the vertical deviation in the trajectory.

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