Numerical analysis of the bubble-particle interaction in an acoustic field

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Abstract. Features of the interaction of a bubble and a solid spherical particle in the presence of an acoustic field in the three-dimensional case are numerically studied using the boundary element method for potential flow. Multiparametric calculations are presented and dependences of the change in the volume of the bubble, dynamics of the mass center of the bubble and particle on the distance between the objects and their sizes are constructed. It is shown that during the bubble expansion, the particle repels from it, and during the bubble shrinkage it is attracted, the size of the particle determines its mobility. On average, over five periods of acoustic field oscillations, the distance between the objects decreases, which is due to the translational motion of the bubble in the compression phase. The features of the deformation of a bubble located near a solid spherical particle with small amplitudes of the acoustic field are studied.

1. Introduction

Oil and gas, medical, environmental, and other industries require the introduction of new technologies that can be developed based on fundamental research in microfluidics. This is due to the fact that the behavior of macrosystems is very complex and is largely determined by hydrodynamic processes at the micro-level, which depend on the shape of the microparticles and their interaction. In this connection, the problem of analyzing the dynamics of individual micro-objects, such as bubbles and solid particles in the field of external forces, remains urgent.

Currently, there are several models describing the interaction of a bubble and a solid particle. In [1], the fifth-order Lagrange equations, which describe the dynamics of a cluster containing spherical bubbles and spherical elastic or solid particles in a potential flow under the influence of an acoustic field or a shock wave, were considered.

In recent years, researchers have begun to use computational fluid dynamics methods to simulate efficiently collisions of bubbles and particles in a flotation machine [2]. Despite the fact that these models are of applied importance in industry, many physical phenomena, such as the movement of bubbles and particles, interfacial forces, and the film drainage process, have not been fully studied. However, accounting for interfacial forces is an important factor in the interaction between a particle and a bubble. In [3], the role of hydrodynamic and surface forces in the interaction of a bubble and a particle was theoretically studied. The authors of [4] calculated the hydrodynamic force acting on the particle from the liquid using a theoretical model. In [5], the process of particle adhesion to the surface of a large air bubble was experimentally studied. The authors of [6] conducted similar experiments to study the trajectory of bubbles on the surface of a large stationary particle. Such studies are important...
for understanding the mechanisms of interaction between a bubble and a particle during the flotation process.

Although there are many works devoted to the bubble-particle interaction, the behavior of a deformable bubble near a solid particle, as well as the hydrodynamic forces arising, have not been fully studied. Besides, in most theories related to the dynamics of bubbles and particles, three-dimensional effects are neglected (e.g., [1]), the deformation of bubbles is not taken into account. In this regard, the development of the mathematical models and the implementation of appropriate program code based on the effective methods and algorithms that describe the combined dynamics of a bubble and a particle in the three-dimensional case are relevant. The authors of the present study successfully used the accelerated boundary element method for studying the dynamics of a bubble cluster [7] in an acoustic field, and implemented the accelerated code based on the boundary element method (BEM) using graphic processors for a cluster containing bubbles and particles [8]. The development and application of the two-dimensional BEM to study the interaction of a solid particle with a bubble that occurs during an underwater explosion, were the focus of modern works [9]. This paper presents a three-dimensional numerical approach based on the BEM for potential flows. The developed approach is used to study the features of the interaction between a bubble and a solid spherical particle under the action of an acoustic field.

2. Problem statement

Consider the dynamics of a bubble (denoted by the subscript “b”) of the volume \( V_b \) bounded by the surface \( S_b \) and a solid particle (denoted by the subscript “p”) of the volume \( V_p \) bounded by the surface \( S_p \) in an unbounded ideal incompressible liquid. The motion of a liquid is described by the Euler equations

\[
\rho_l \frac{dv}{dt} = -\nabla p + \rho_l g, \quad \nabla \cdot v = 0, \quad \frac{d}{dt} \frac{\partial}{\partial t} + v \cdot \nabla,
\]

where \( g \) is the vector of gravitational acceleration, \( p, v \) and \( \rho_l \) are the pressure in the liquid, velocity and density, respectively. Further, we will assume that the liquid is at rest at infinity. The pressure at infinity is determined according to the acting acoustic field \( P(t) = P_0 + P_a \sin(\omega t) \), where \( P_0, P_a, \omega \) are the initial pressure in the liquid, the amplitude and cyclic frequency of the acoustic field, respectively.

We denote the radius vectors of points on the surfaces \( S_b \) and \( S_p \) by \( \mathbf{r}_b \) and \( \mathbf{r}_p \), and the normals to these points (directed into the liquid) by \( \mathbf{n}_b \) and \( \mathbf{n}_p \), respectively. Thus, we can write the kinematic conditions on the surface of the bubble and particles

\[
\mathbf{n}_b \cdot \mathbf{v} \mid_{r=r_b} = \mathbf{n}_b \cdot \frac{d\mathbf{r}_b}{dt}, \quad \mathbf{n}_p \cdot \mathbf{v} \mid_{r=r_p} = \mathbf{n}_p \cdot \frac{d\mathbf{r}_p}{dt}.
\]

We assume that the gas inside the bubble behaves polytropically with the polytropic exponent \( \kappa \), then the pressure at the bubble boundary is calculated by

\[
p \mid_{r=r_b} = p_g - 2\gamma k, \quad p_g = p_{g0} \left( \frac{V_{00}}{V_b} \right)^\kappa,
\]

where \( \gamma \) is the coefficient of surface tension, \( k \) is the average curvature of the surface, \( p_{g0} \) is the pressure in the gas (the index «0» denotes the initial state).
The dynamics of a solid particle can be described as follows. We denote the coordinates and the velocity of the center of mass of the particle as \( R_p \) and \( V_p \), respectively. Then the translational velocity of a spherical particle can be written as

\[
\frac{dR_p}{dt} = V_p. \tag{3}
\]

To close the system of equations, it is necessary to calculate the force acting on the particle, which has two components, including mass and surface forces

\[
F_p = m_p g - \int_{S_p} p n dS. \tag{4}
\]

In addition, it is assumed that the flow is potential, that is, \( \mathbf{v} = \nabla \phi \), where \( \phi \) is the velocity potential that satisfies the Laplace equation \( \nabla^2 \phi = 0 \). Then equation (1) for a liquid resting at infinity can be rewritten in the form of the Cauchy-Lagrange integral, and the velocity potential at the boundary of the bubble and particle is determined according to the dynamic condition

\[
\frac{d\phi}{dt} = \frac{1}{2} |\nabla \phi|^2 - \frac{p}{\rho_l} + g \cdot r|_s + P(t). \tag{5}
\]

Then the kinematic boundary conditions (2) in the case of a potential flow are written as follows

\[
\frac{\partial \phi}{\partial n} \bigg|_{r=r_0} = n_p \cdot \frac{dr_p}{dt}, \quad \frac{\partial \phi}{\partial n} \bigg|_{r=r_p} = n_p \cdot \frac{dr_p}{dt}. \tag{6}
\]

Substituting in the formula (4) the pressure expressed in terms of the velocity potential in accordance with the Cauchy-Lagrange integral (5) we obtain

\[
F_p = (\rho_p - \rho_l) V_p g + \rho_l \int_{S_p} \left( \frac{\partial \phi}{\partial t} + \frac{1}{2} |\nabla \phi|^2 \right) n dS. \tag{7}
\]

Using (2), the equation of the particle motion can be written in the boundary-integral form

\[
\frac{dV_p}{dt} = (1 - \frac{\rho_l}{\rho_p}) g + \frac{\rho_l}{m_p} \int_{S_p} n \phi dS + \frac{1}{2} \int_{S_p} \left( \frac{\partial \phi}{\partial n} \cdot \nabla \phi \right) n dS. \tag{8}
\]

By entering a new variable

\[
U_p = V_p - \frac{\rho_l}{m_p} \int_{S_p} \phi n dS \tag{9}
\]

boundary-integral equation (8) can be rewritten in the form

\[
\frac{dU_p}{dt} = \left( 1 - \frac{\rho_l}{\rho_p} \right) g + \frac{\rho_l}{m_p} \int_{S_p} \left( \frac{1}{2} |\nabla \phi|^2 \right) dS. \tag{10}
\]

Relation (6) taking into account (6) and (9) can be reduced to the form
Equation (11) allows us to exclude the normal derivative of the velocity potential \( q \) to the particle surface and leads to the boundary integral equation, described in [8]. If the velocity potential values \( \phi_b \) on the bubble surface at the corresponding points are known, the unknown values of the normal derivative of the velocity potential \( q_b \) on the bubble surface and velocity potential \( \phi_p \) on the particle surface can be found from integral equation [8]. Thus, the problem reduces to solving a system of ordinary differential equations (ODE) (5) and (6) for the bubble dynamics, (3) and (10) for the particle motion, which are solved at the first time steps by the fourth-order Runge-Kutta method, and then method of Adams-Bashfort of the 4th order.

3. Analysis of the numerical results

We considered the interaction of a bubble and a solid spherical particle (\( \rho_p = 2000 \text{ kg/m}^3 \)) with characteristic size \( r_0 = 10 \mu m \) in water (\( \rho_l = 1000 \text{ kg/m}^3 \), \( \kappa = 1.4 \), \( \gamma = 0.073 \text{ N/m} \)) in the presence of an acoustic field (\( P_a = 0.5 p_0 \), \( p_0 = 0.1 \text{ MPa} \), \( \omega / (2\pi) = 200 \text{ kHz} \)). At the initial moment of time, the center of the bubble coincided with the origin \( R_b = (0,0,0) \), and the particle center lays at the point \( R_p = (d,0,0) \) from the bubble center at distance \( d \).

The convergence and accuracy of program code are demonstrated for the interaction of a bubble and a solid particle of the same radius \( r_{00} = r_p = r_0 \), located at the distance \( d_0 = 12r_0 \), where \( r_{00} \) is the initial radius of the bubble, \( r_p \) is the particle radius. Numerical results and the solution of the Rayleigh-Plesset equation are good agreement for the radius dynamics of a single spherical bubble in an acoustic field without taking into account the viscosity of the liquid. The relative error in the space L∞ for number of calculation points \( N = 642 \) is 2.31%.

Multiparametric calculations are conducted for bubbles and spherical particles of various radii located at different distances from each other. In the first case, we considered a bubble and a particle of radius \( r_{00} = r_p = r_0 \) located at a different distance from each other. The analysis shows that the change in the volume of the bubble does not depend on the distance, however, with a decrease in the distance between the centers of the objects, the deviation from the initial position is more significant. During bubble shrinkage, the disperse objects are attracted to each other, while the bubble extends they repel from each other, which is associated with the formation of hydrodynamic flows created by the oscillating bubble. On average, over 5 periods of the acoustic field, the distance between the objects decreases, which is explained by the translational motion of the bubble in the shrinkage phase.

Figure 1 (a,b,c) shows the results of multiparametric calculations depending on the size of the bubble for \( d_0 = 4r_0 \). It can be seen from the figure that the size of the bubble significantly affects the change in its volume (a), and the oscillations of the bubble determine the translational motion of the particle (b) and the bubble (c). As in the first case, in the shrinkage phase, the objects are attracted to each other, in the expansion phase, the particle repels from the bubble, and on average over 5 periods the distance between the objects decreases. The larger the size of the bubble, the greater the amplitude of its oscillations. Thus, the greatest deviation of objects from the initial position is achieved with a bubble radius 2 times larger than the particle size.

We also conducted an analysis of the deformation of a bubble of radius \( r_{00} = r_0 \) located at the origin \( R_b = (0,0,0) \) (Figure 2) and with a displacement along the y axis to the point \( R_p = (0,r_0,0) \) (Figure 3), near a solid spherical particle of radius \( r_p = 3r_0 \), located at a distance \( d_0 = 5r_0 \) from the
center of the coordinate system in the direction of the x axis. Figures 2 and 3 show the projection of the bubble and particle shape in the Ox’y’ plane (a) and three-dimensional visualization (b) at various points in time, where x’ and y’ are the coordinates related to the characteristic size of the problem r₀.

According to Figure 2, in the shrinkage phase (t₁=2.698T) the bubble stretches along the y axis, and in the expansion phase (t₃=3.098T) along the x axis, where T is the acoustic field period. However, the symmetry of the bubble shape along the x axis is lost when the bubble is displaced by one characteristic size along the y axis (Figure 3). In this case, symmetry is observed relative to the line of the centers of objects, and in this case, the nature of the dynamics of the bubbles shown in Figures 2 and 3 is the same.

Figure 1. The dynamics of the bubble volume (a,d), the center of mass of the solid particle (b,e), and the center of mass of the bubble (c,f) depending on the initial radius of the bubble (left side with black lines) and on the radius of the particle (right side with gray lines).

Figure 2. Deformation of the bubble with R₀ = (0,0,0) (gray color) near the particle (black color) in the Ox’y’ plane (a) and in the three-dimensional case (b).
Conclusions
Based on the three-dimensional boundary element method for potential flows, the dynamics of the bubble and particle in an acoustic field are studied. The dependences of the change in the center of mass of the bubble and particle, as well as the volume of the bubble on the distance and size of objects are presented. It is revealed that when the bubble expands, the particle repels from it, while the bubble shrinks, disperse objects are attracted. This is explained by the formation of hydrodynamic flows created by the oscillating bubble, which are directed towards the particle during bubble expansion, and towards the bubble during its shrinkage. It is also found that in the shrinkage phase the bubble progressively moves towards the particle.

Figure 3. Bubble deformations with $\mathbf{R}_b = (0, r_0, 0)$ (gray color) near the particle (black color) in the Ox’y’ plane (a) and in the three-dimensional case (b).

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