Mathematical model of the flotation complex particle–bubble within the framework of Lagrangian formalism

N P Moshkin\textsuperscript{1,3} and S A Kondratiev\textsuperscript{2}

\textsuperscript{1} Lavrentyev Institute of Hydrodynamics, 630090 Novosibirsk, Russia
\textsuperscript{2} Chinakal Institute of Mining, 630091 Novosibirsk, Russia
\textsuperscript{3} Novosibirsk State University, 630090 Novosibirsk, Russia

E-mail: nikolay.moshkin@gmail.com

Abstract. A model of the interaction of a spherical gas bubble and a rigid particle is derived as a coupled system of second-order differential equations using Lagrangian mechanics. The model takes into account oscillations of the bubble surface and the attached to it solid cylindrical particle in infinite volume of ideal incompressible liquid. The capillary force holding the particle on the bubble is due to the shape of the meniscus surface, which determines the wetting edge angle. The series with respect Legendre polynomials is used to present small axisymmetric oscillations of the particle-bubble system. Potential and kinetic energies are expressed through coefficients of this series. Particle adhesion condition to bubble surface is implemented through Lagrange multipliers. The dependence of the particle size and its density is demonstrated as a result of the numerical integration of the resulting dynamic system of differential equations.

1. Introduction
The behavior of the gas bubble to which a small solid particle is attached is of practical interest in the flotation process during the enrichment of mineral ores. The eigenmodes of axisymmetric oscillations of a gas bubble in an inviscid fluid have been derived by Rayleigh [1].

A bubble with attached a solid particle behaves differently from a free bubble or a bubble that is in contact with a solid support. In this case, unlike free behavior, an additional low-frequency mode of oscillation may appear. In practice, the smallest non-zero frequency mode is important, since it is usually the most expected. The present work is devoted to the study of the effect of a heavy particle attached to bubble surface. An oscillating bubble and a heavy particle are considered as a single mechanical system subject to geometric coupling (the particle is located on the bubble surface in the lower position – relative to the direction of the gravity vector).

2. Math statement of problem
Suppose that the small gas bubble, together with the particle attached to it, are in a non-viscous incompressible liquid of infinite extent. The equation of the bubble surface in the spherical coordinate system associated with the center of the bubble is written in the form, $r = R + \eta(t, \mu)$, where $R$ is the unperturbed radius of the bubble, $\mu = \cos(\theta)$ and the angle $\theta$ is counted from the upper part of the vertical axis, $\eta(t, \mu)$ is surface perturbation, which is
assumed to be axisymmetric and small. The perturbation can be represented by the series with respect to the Legendre polynomials $P_j(\mu)$ of order $j$

\[ \eta(t, \mu) = \sum_{j=0}^{N} b_j(t) P_j(\mu). \]

Coefficients $b_j(t), \ j = 0, 1, ..., N$ are the “generalized” coordinates of the bubble surface. The cylindrical particle of the mass $m_p$, density $\rho_p$, radius $r_0$ and height $h$ is attached to the bubble surface and is held by the capillary force acting along the three-phase contact line of the particle. The particle is attached at position $\theta_0 = 180^\circ$ and can oscillate in radial direction. Figure 1 shows a solid particle adhering to a free gas-liquid interface, corresponding to a bubble having an infinitely large radius. Let’s accept assumptions, 1) $r_0/a = o(1), h/a = 0(1)$, here $a = \sqrt{\sigma/(\rho fg)}$

is the capillary constant, $\sigma$ is the surface tension, $\rho_f$ is the fluid density, $g$ is the gravity acceleration; 2) the surface of the bubble is “flat” near the contact zone with the particle, i.e. the radius of the bubble $R$ is an order of magnitude greater than the radius of the particle. Under these assumptions, as shown in [2], the surface of the meniscus $z = z(\theta)$ is described by the Laplace equation. The expression

\[ z(\theta) = K_0 r_0 \tan(\theta) \]  

showed a good agreements with the experiments [3], where $K_0 = -\ln(r_0/2a) - \gamma$ and $\gamma = 0.5772$ is the Euler’s constant. The position of the particle is determined by the “generalized” coordinate $z(t) = b_{N+1}(t), \ (R+b_{N+1}(t))$. At the initial moment, the position of the particle coincides with the surface of the bubble. At further moments, the particle remains on the surface of the bubble and moves only in radius

\[ g(b_1, \ldots, b_N, b_{N+1}, t) = \sum_{j=0}^{N} b_j(t) P_j(\mu_0) - b_{N+1}(t) = 0. \]

The latter equation imposes a constrain on the generalized coordinates $b_j(t), \ j = 0, 1, ..., N + 1$ of the mechanical system in question consisting of a bubble with an attached particle in position $\mu_0 = \cos(\theta_0)$

The potential energy of the system consists of the following components: a) the interfacial energy, $\sigma \Delta s$, there $\Delta s$ is interfacial area increases, b) the potential energy of the particle. The potential energy of the particle associated with gravity can be omitted. One assume that only capillary force acts on the particle, $F = 2\pi \sigma r_0 \sin \theta$. The change in the potential energy of the particle has the form

\[ U_p = F \cdot z = 2\pi \sigma r_0 \sin(\theta) \cdot z = 2\pi \sigma r_0^2 K_0 \sin(\theta) \cdot tg(\theta) = 2\pi \sigma r_0^2 K_0 \frac{tg^2(\theta)}{\sqrt{1 + tg^2(\theta)}}. \]

Figure 1. The cylindrical particle of the mass $m_p$, density $\rho_p$, radius $r_0$ and height $h$ is attached to the bubble of infinitely large radius. $\theta$ is the three-phase contact angle, $F$ is the capillary force, $z(\theta)$ is the equation of meniscus.
Using (1) one obtains that \( z' = (tg(\theta))'K_0r_0 \), and therefore it is possible to write down the kinetic energy of the moving particle \( T_p = \frac{m_p(z')^2}{2} = \frac{m_p((tg\theta)')^2}{2}K_0^2r_0^2 \). Denoting \( y = r_0 \tan(\theta) \) one get

\[
T_p = \frac{m_pK_0^2(y')^2}{2}, \quad U_p = 2\pi\sigma K_0r_0 \frac{y^2}{\sqrt{r_0^2 + y^2}}.
\]

Following the work [4] the potential energy due to the elastic force of the bubble surface and the kinetic energy (the kinetic energy of a liquid outside the bubble) are

\[
U_f = 2\pi\sigma \sum_{j=2}^{N} \frac{j^2 + j - 2}{2j + 1}b_j^2(t), \quad T_f = 2\pi R^3 \rho_f \sum_{j=1}^{N} \frac{1}{(j + 1)(2j + 1)}b_j^2(t).
\]

A point above the symbols denotes a time derivative. The force of gravity and dissipation of energy into heat is not taken into account.

### 2.1. Lagrange equation

Lagrangian in terms of the kinetic and potential energies of the system is \( L = L_f + L_p = (T - U)_f + (T - U)_p \).

\[
L_f = 2\pi R^3 \left[ \rho_f \sum_{j=1}^{N} \frac{1}{(j + 1)(2j + 1)}b_j^2(t) \right] - 2\pi\sigma \sum_{j=2}^{N} \frac{j^2 + j - 2}{2j + 1}b_j^2(t), \quad (4)
\]

\[
L_p = \frac{m_pK_0}{2}y^2 - 2\pi\sigma K_0r_0 \frac{y^2}{\sqrt{r_0^2 + y^2}} - m_p \sum b_jP(\mu_0) \bigg| yK_0. \quad (5)
\]

The last term in (5) appears since the particle is tied to the moving surface of the bubble (i.e., the coordinate system is non-inertial). The resultant Lagrangian is then used to formulate the Euler- Lagrange equations

\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{b}_j} - \frac{\partial L}{\partial b_j} = \lambda \frac{\partial g}{\partial b_j}, \quad j = 1, \ldots, N + 1; \quad g(b_1, \ldots, b_N, b_{N+1}, t) = 0.
\]

Here, \( \lambda \) is the Lagrange multiplier that allows one to take into account the constraint (2). So one has \( N + 2 \) equations and \( N + 2 \) unknowns. The result is a system of nonlinear differential equations. From this system the equations governing the bubble shape oscillations and the particle motion are obtained, and are given in terms of the variable \( y \) (but one can return to \( z \)).

\[
4\pi R^3 \rho_f \frac{\ddot{b}_j}{(j + 1)(2j + 1)} + 4\pi\sigma \frac{j^2 + j - 2}{2j + 1}b_j(t) = \pm \lambda P_j(\mu_0); \quad j = 2, \ldots, N;
\]

\[
m_pK_0^2\dddot{y} + 2\pi\sigma K_0r_0 \left[ 2 - \frac{y}{\sqrt{r_0^2 + y^2}} - \left( \frac{y}{\sqrt{r_0^2 + y^2}} \right)^3 \right] + m_pK_0 \left[ \sum b_jP(\mu_0) \right] = \mp \lambda K_0, \quad (6)
\]

\[
\sum_{j=1}^{N} b_j(t)P_j(\mu_0) - K_0y = 0, \quad \left[ - \sum_{j=1}^{N} b_j(t)P_j(\mu_0) + K_0y \right] = 0.
\]

Recast the system of equations (6) in dimensionless form (values with “*” dimensionless)

\[
t^* = \sqrt{\frac{\sigma}{\rho_f R^3}}, \quad b^* = \frac{b}{R}, \quad y^* = \frac{y}{R}, \quad \lambda^* = \frac{1}{4\pi} \frac{\lambda}{R^2}\sigma,
\]

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here the characteristic period of oscillations \( \left( \frac{\rho_f R^3}{\sigma} \right)^{1/2} \) is used as a time scale. Equations using dimensionless values have the following form

\[
\begin{align*}
\frac{\ddot{b}_j}{(j+1)(2j+1)} + \frac{j^2 + j - 2}{2j+1} b_j(t) &= \pm \lambda P_j(\mu_0); \quad j = 1, 2, \ldots, N; \\
\frac{K_0}{3} \frac{m_p y_j}{m_{fl}} + \frac{r_0}{R} \left( \frac{y_j}{\sqrt{r_0^2 + y_j^2}} \right)^3 - \frac{1}{2} \left( \frac{y_j}{\sqrt{r_0^2 + y_j^2}} \right)^3 + \frac{m_p K_0}{3} \left[ \sum b_j P(\mu_0) \right] &= \mp \lambda K_0, \\
\sum_{j=1}^{N} b_j(t) P_j(\mu_0) - K_0 y &= 0, \\
\left[ -\sum_{j=1}^{N} b_j(t) P_j(\mu_0) + K_0 y \right].
\end{align*}
\]

There are three dimensionless parameters \( K_0 \) which appears in (1), ratio of the particle mass to the mass of fluid in the volume of bubble \( m_p/m_{fl} \) and the ratio of particle and bubble radius. Using a constraint (2), one can exclude \( \lambda \)

\[
\lambda = \frac{3}{2} \frac{m_{fl} r_0}{m_p} \left( \frac{y_j}{\sqrt{r_0^2 + y_j^2}} \right)^3 - \frac{1}{2} \left( \frac{y_j}{\sqrt{r_0^2 + y_j^2}} \right)^3 - \frac{1}{2} \left( \frac{y_j}{\sqrt{r_0^2 + y_j^2}} \right)^3 + \frac{3 m_{fl}}{2 m_p}.
\]

As a result, one obtain an ODE system for vectors \( b_j(t), j = 1, \ldots, N + 1 \) and \( y \),

\[
\begin{align*}
\dot{b}_j &= -\lambda(t)(j+1)(2j+1)P_j(\mu_0) - (j+1)(j^2 + j - 1)b_j, \\
\dot{y} &= \frac{3}{2} \frac{m_{fl} r_0}{K_0 m_p} \lambda(t) - \frac{3}{2} \frac{m_{fl} r_0}{K_0 m_p} R \left( \frac{y_j}{\sqrt{r_0^2 + y_j^2}} \right)^3 - \frac{1}{2} \left( \frac{y_j}{\sqrt{r_0^2 + y_j^2}} \right)^3.
\end{align*}
\]

The solution of the system of differential equations (7) requires the setting of initial data for functions and their first derivatives. The values of the derivatives must be matched with the restriction (2) (the particle is on the surface of the bubble). Let the initial data be set as follows

\[
\begin{align*}
\dot{b}_j(0) &= b_{0j}, \quad y(0) = \frac{1}{K_0} \sum b_j(0) P_j(\mu_0), \\
\dot{y}(0) &= \dot{b}_{0j}, \quad \dot{y}(0) = \frac{1}{K_0} \sum \dot{b}_j(0) P_j(\mu_0).
\end{align*}
\]

One only needs to specify coefficients \( b_j(0), \dot{b}_j(0), j = 1, \ldots, N + 1 \). The bubble and particle behavior is entirely characterized by the equations motion (7)–(8). The dynamic shape and particle oscillations are obtained from these equations using standard methods.

3. Results and discussions

The computational solutions of equations (7), (8) are carried out to estimate oscillations of the particle and the bubble surface perturbations. It is evident that in any numerical study a vast number of possibilities can be considered. Here we conduct a preliminary study only try to demonstrate how an initial perturbation in a low order shape modes causes system behavior. Calculations were made at values of parameters close to real physical dimensions of gas bubble and flotated particle. In particular \( R = 0.00052(m), \rho_p = 4500kg/m^3, \rho_f = 1000kg/m^3, \)

\[
\sigma = 0.072N/m, \quad h = 0.0015 - 0.0025m.
\]
Calculation results are given in figures 2–5. Figure 2 shows the particle oscillations near the equilibrium position \( z = 0 \) for two different initial velocities, \( \dot{b}_0 = 0.1 \text{m/s} ; 0.5 \text{m/s} \) (8). All other components \( b_{0j} \) were zero. Figure 3 shows deviations of liquid gas boundary from horizontal depending on time. Dashed lines correspond to initial velocity \( 0.1 \text{m/s} \) and solid lines correspond to velocity \( 0.5 \text{m/s} \).

Figure 2. Particle oscillation near \( z = 0 \) as function of time. \( r_0 = 100 \mu m, h = 150 \mu m \).

The particle oscillates close to harmonic. Figure 4 presents the particle oscillation predicted for the two different heights \( h = 150 \mu m \) (dashed line) and \( h = 250 \mu m \) (solid line). With an increase in particle size (for example, cylinder mass due to an increase in its height), an increase in oscillation amplitude and phase shift are observed. Figures 2–4 present the results predicted for perturbation only the second mode \( b_2(t) \) at the initial instant. In order to understand the interaction between modes, Figure 5 presents computational results for an initial perturbations in the \( n = 2 \) and \( n = 3 \) shape modes \( b_{02} = 10^{-4} \text{m}, b_{03} = 10^{-4} \text{m}, \dot{b}_{02} = 0.1 \text{m/s}, \dot{b}_{03} = 0.01 \text{m/s} \). Oscillation patterns are more complex and non-harmonic.

Figure 3. Angle \( \theta \) — deviations of liquid gas boundary from horizontal depending on time. \( r_0 = 100 \mu m, \dot{b}_{02} = 0.1 \text{m/s}, h = 150 \mu m \).

Figure 4. Predicted particle oscillation. \( r_0 = 100 \mu m, \dot{b}_{02} = 0.1 \text{m/s} h = 150 \mu m \) — dashed line, \( h = 250 \mu m \) — solid line.

Figure 5. Predicted particle oscillation in case where at the initial time the two modes are perturbed. \( b_{02} = 10^{-4} \text{m}, b_{03} = 10^{-4} \text{m}, \dot{b}_{02} = 0.1 \text{m/s}, \dot{b}_{03} = 0.01 \text{m/s} \).
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