Modelling the motion of a collected particle over a bubble surface

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Abstract

Froth flotation is a process that utilizes the surface properties of mineral particles to separate them from unwanted gangue materials. Usually, the mineral particles are either naturally hydrophobic, or surfactant-treated hydrophobic and thus, they are prone to adhere to bubbles. Once attached, the capillary force is dominant in the control of the particle bubble aggregate stability. Capillary force is a function of surface tension and contact angle, which is a measure of particle hydrophobicity. In this paper, the Discrete Element Method has been applied to simulate the interaction between particles and a central bubble in a quiescent liquid with the aim of describing: (1) the motion of the particle sliding over the bubble surface, and (2) the formation of the three phase contact line. Simulation results for particle-bubble separation distance versus time showed excellent agreement with experimental observations. Moreover, the simulations correctly predicted the time when the particle contacted the bubble. Additional simulations were carried out for multi-particle attachment that highlighted the interaction between particles, including collision and rebounding phenomena. These simulations correctly captured experimental observations reported in the literature and have provided valuable insight into the particle loading capacity of bubbles being utilized in mineral flotation devices.

Keywords: Particle bubble interaction; particle penetration; particle collision; Discrete Element Method (DEM)

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1. Introduction

Froth flotation is an important industrial process that has been extensively used for a long time in the separation of mineral particles. During processing, hydrophobic particles will attach to air bubbles passing through the particle suspension and, consequently, rise to the top of the surface together, leaving the undesirable materials (gangue which is hydrophilic) in the bulk liquid. Given the industrial importance of froth flotation, considerable information has been gained from previous studies focusing on surfactants used in flotation process [1, 2] as well as particle-bubble interactions [3-5]. On the basis of these studies, it is believed that the satisfactory improvement in the performance of the froth flotation process depends on providing adequate understanding of the interactions between particles and bubbles as well as detailed knowledge of the interacting forces which govern the dynamics at each stage of the process.

Particle-bubble interaction is generally considered to involve collision, attachment and detachment [6-8]. The collision involves the approach of a particle to an air bubble surface, which is subjected to the effect of liquid hydrodynamics of fluid flows in the bulk as well as in the thin intervening liquid film between the particle and the bubble. When the particle and the bubble are in close proximity, the intervening liquid film tends to thin to a critical value of rupture leading to the formation of three-phase contact line (TPCL). This is followed by the expansion of the TPCL until an equilibrium wetting perimeter is formed. These phenomena are referred to as the process of attachment. If the particle is too heavy or the turbulent intensity of the fluid is high enough so the capillary force is not sufficiently strong to hold the attached particle, the detachment of the particle from the bubble will result [3,8].

With the aid of the surface forces apparatus and, more recently, the atomic force microscope, a large amount of experiments have been conducted to study particle-bubble interactions in stationary liquid [3-5]. However, due to the complexity of the flotation phenomenon, the principles governing bubble-particle interactions are not fully understood despite many decades of research.

Alternatively, numerical simulations become highly recommended for such complicated study, owing to the fast advancement in computational capability and the rapid emergence of advanced numerical methods nowadays. Discrete Element Method (DEM), since being introduced in the 1970s [9], has become a powerful tool for investigating the detailed particle phenomena. In this method, all particles are explicitly considered as individual bodies each governed by Newton’s second law of motion. A small overlap is allowed between contacting particles, which is considered as particle deformation and therefore result in an elastic force between them. The evolution of the system is advanced in an explicit manner using sufficiently small time steps. It is possible to include both macroscopic (drag force, buoyancy force, capillary force etc.) and microscopic (van der Waals force, electrical double-layer force, hydrophobic force, etc.) physics in the DEM framework to model the particle-particle interactions in a more realistic way. For such reasons, DEM can be applied to simulate particle-bubble system by simply considering the bubble as an elastic body [10, 11]. Such simulation of bubble-particle interactions is significant in industrial applications like mineral recovery by flotation process which can benefit from enhanced recovery once the bubble-particle interactions are well understood.

In this work, we present a detailed three-dimensional DEM model for particle-bubble interactions operating in a quiescent liquid. Specifically, a preliminary experimental validation of the DEM model is reported in terms of interactions between a single particle and a stationary air bubble. The model is then extended to the study of multi-particle – single bubble interactions.

2. Numerical methodology

2.1. Numerical modeling of single particle-bubble system using Schulze’s theory

Under quiescent conditions, the dynamic motion of an attached particle on a stationary bubble surface can be modelled according to the theory proposed by Schulze [6]. Various forces acting on the particle in this case include the gravity \( F_G \), buoyancy \( F_B \), surface tension \( F_S \), pressure force \( F_P \), and hydrodynamic drag \( F_D \). Descriptions of each of these forces are given below.
- **Gravitational and buoyancy forces.** A particle of finite mass immersed in fluid experiences a net buoyancy force in the direction opposite of gravitational acceleration which is expressed as:

\[ \mathbf{F}_G + \mathbf{F}_B = \frac{4}{3} \pi R_p^3 (\rho_p - \rho_l) \mathbf{g} \]  

(1)

where \( R_p \) is the radius of particle, \( \mathbf{g} \) is the gravitational acceleration and, \( \rho_p \) and \( \rho_l \) are the particle and liquid densities respectively. We note that the volume of the particle in the air phase is assumed to be very small that there is no diminishment in the buoyancy and gravity of the particle, therefore, Eq. (1) is maintained for the attached particle.

- **Surface tension force.** When the particle attaches on the bubble interface, the intervening liquid film at the solid-liquid interface drains off developing a three phase contact line and the corresponding surface tension force. This force can be expressed as:

\[ \mathbf{F}_{ST} = -2\pi \sigma R_p \sin \alpha \sin(\theta - \alpha) \mathbf{n} \]  

(2)

where \( \sigma \) is the gas-liquid surface tension, \( \alpha \) is the filling angle measured from the bubble-particle centreline to the connecting line of particle centre to the three phase contact, \( \theta \) is the contact angle, and \( \mathbf{n} \) represents the unit vector directing from the centre of the bubble to the centre of particle. In the implementation, \( \alpha \) is calculated based on the assumption that the local distortion of the bubble surface is negligible. Accordingly, we could obtain an estimate for this angle by performing the law of cosine to the triangle with three sides of the radii of particle and bubble, \( R_p \), \( R_b \), and the distance between particle and bubble centres, \( d \).

- **Pressure force.** The internal pressure (Laplace pressure) of the bubble is higher than the surrounding pressure of the liquid phase. Taking into consideration the depression of bubble interface at bubble-particle contact, and then subtracting the hydrostatic head, the net pressure force acting on the solid-gas contact area is given by:

\[ \mathbf{F}_p = \pi R_p^2 \sin^2 \alpha \frac{2\sigma}{R_b} - \rho_l g \frac{Z}{h} \]  

(3)

where \( Z \) is the height difference between the bubble apex and the centre of the TPCL. Expression (3) is valid under the assumption of the plane of TPCL being considered as a point.

- **Drag force.** Under the condition of creeping flow, the drag force experienced by the particle is given by Stokes law as:

\[ \mathbf{F}_D = -6\pi \mu R_p \mathbf{v} \]  

(4)

where \( \mu \) is the liquid viscosity, and \( \mathbf{v} \) is the particle velocity.

Incorporating all the above described force into the equation of motion of the particle in two dimensions using Newton’s second law can be described as follows:

\[ m_p \frac{dv_x}{dt} = \sum F_x = -6\pi \mu R_p v_x - 2\pi \sigma R_p \sin \alpha \sin(\theta - \alpha) n_x + \pi R_p^2 \sin^2 \alpha \frac{2\sigma}{R_b} - \rho_l g \frac{Z}{h} n_x \]  

(5a)

\[ m_p \frac{dv_y}{dt} = \sum F_y = 4(\rho_v - \rho_p) \pi R_p^2 g_y - 6\pi \mu R_p v_y - 2\pi \sigma R_p \sin \alpha \sin(\theta - \alpha) n_y + \pi R_p^2 \sin^2 \alpha \frac{2\sigma}{R_b} - \rho_l g \frac{Z}{h} n_y \]  

(5b)
where \( m_p \) is the particle mass, \( n_x \) and \( n_y \) are two components of unit vector, \( \mathbf{n} \), in \( x \) and \( y \) directions respectively. In order to apply Eq. (5a) and (5b), it is convenient to transform the vector \( \mathbf{d} = d\mathbf{n} \) from Cartesian to spherical coordinates \((r, \phi)\), where \( r \) is the displacement of the particle’s centre from the bubble’s centre (the origin) and \( \phi \) is the polar angle measured out from the horizontal ordinate. The transformation yields \( Z = R_b(1 - \sin \phi) \), \( n_x = \cos \phi \) and \( n_y = \sin \phi \). Eq. (5a) and (5b) were numerically solved using a MATLAB in-built solver, ode113, which is a multistep variable order Adams-Bashforth-Moulton PECE (Predict–Evaluate–Correct–Evaluate) solver with time step size of \( 10^{-5} \) s.

2.2. Numerical modelling of particle-bubble system using complete DEM model

It is worth noting that the numerical model developed based on Schulze’s theory for quiescent condition in the previous section does not consider all the necessary forces required for complete description of bubble-particle interaction physics. In addition to the forces considered before, few other forces namely hydrophobic force \((\mathbf{F}_H)\), hydrodynamic resistance force \((\mathbf{F}_{HR})\) and normal contact force \((\mathbf{F}_{NC})\) were accounted for to develop a complete DEM model (Discrete Element Modelling).

In the model, the bubble was assumed to be a stationary spherical elastic body and no liquid flow was considered, which simplifies the simulations and the model analysis significantly. The equation of motion for a frictionless spherical particle is given based on Newton’s second law of motion:

\[
\frac{m_p}{t} \frac{d\mathbf{v}}{dt} = \mathbf{F}_{\text{total}}
\]

\[
\mathbf{F}_{\text{total}} = \mathbf{F}_G + \mathbf{F}_B + \mathbf{F}_{ST} + \mathbf{F}_P + \mathbf{F}_{HR} + \mathbf{F}_H + \mathbf{F}_{NC}
\]

where \( \mathbf{F}_{\text{total}} \) is total external forces. In the DEM model, the effect of net DLVO (Derjaguin, Landau, Verwey, and Overbeek) force, i.e., van der Waals and electrical double-layer forces was ignored.

Since most of the forces were discussed in the previous section, only these additional forces are described here:

- **Hydrodynamic resistance force.** The hydrodynamic resistance could significantly affect the particle-bubble interactions at short separation distances, which is modelled by simply introducing a correction factor to the drag force in both radial and tangential directions.

\[
\mathbf{F}_{r-D} = -6\pi\mu R_p \mathbf{v}_{r-slip} f_1
\]

\[
\mathbf{F}_{t-D} = -6\pi\mu R_p \mathbf{v}_{t-slip} f_3
\]

where the subscripts ‘\( r \)’ and ‘\( t \)’ mean the radial and tangential components, \( \mu \) is the viscosity of a quiescent fluid, \( \mathbf{v}_{\text{slip}} \) describes the relative velocity of the particle with respect to the liquid (slip velocity), \( f \) is the hydrodynamic resistance function and its subscripts identify each problem. For the case, when a particle is moving in a boundless stationary fluid, \( f_1 = f_3 = 1 \) which gives the Stokes drag force, while for the situation where the particle is approaching a bubble surface that can be considered locally planar and immobile, the resistance functions are then given by [8]:

\[
f_1 \approx \left[ 1 + \left( \frac{R_p}{H} \right) ^{0.89} \right] ^{1.124}
\]
where \( H \) is the surface-to-surface separation distance. To avoid the numerical problem that both \( f_1 \) and \( f_3 \) tend to reach infinity when \( H = 0 \), a cut-off distance of 5Å is used herein [10,11]. That is, if the separation is larger than the cut-off distance, Eq. (10) and (11) hold; otherwise, the resistance functions will be evaluated to be one (corresponding to Stokes drag). It is important to note that, to exactly calculate this drag on an attached particle, one need to have the knowledge of the flow-field around the particle with the presence of the gas-liquid interphase; however, such a calculation is beyond the scope of our current work. Instead, we simply assumed the Stokes drag force acting on the attached particle.

- **Hydrophobic force.** When a hydrophobic particle approaches the bubble surface to a close proximity around a few nanometers, the DLVO forces fail to describe their interactions because of non-DLVO forces coming into play [8]. Hydrophobic force is considered to be the most significant non-DLVO force that determines the capture of a particle by a rising bubble during flotation [12]. Till recently, there is no generally accepted mathematical expression to account for this force. In the present study, an exponential form [13] was adopted, which is described as:

\[
F_H = -KR_p \exp\left(-\frac{H}{\lambda}\right)
\]  

where \( K \) and \( \lambda \) are the pre-exponential parameter and exponential decay length, respectively. Again, the same cut-off distance (5Å) is used in this calculation where the hydrophobic force reaches the maximum value, \( F_{H_{\text{max}}} \), that was given beforehand as an input parameter.

- **Normal contact forces.** The contact forces due to a collision of a pair of spheres are computed based on the amount of overlapping of these two contacting bodies. The contact force-displacement relation used herein is based on the linear spring-dashpot model [9].

\[
F_{NC} = k\delta - \eta v_r
\]

\[
\eta = -\eta_{cr} \ln e / \sqrt{\pi^2 + (\ln e)^2}, \quad \eta_{cr} = 2 \frac{m_1m_2k}{m_1 + m_2}
\]

where \( k \) is the stiffness of contact, \( \delta = R_p + R_b - d \) is the overlap of the two spherical surfaces of contact, \( \eta \) is the damping coefficient which is proportional to the critical damping, \( \eta_{cr} \), for the system of two rigid bodies with masses \( m_1 \) and \( m_2 \), and \( e \) is the restitution coefficient. As shown in Eq. (13), the first term on the right hand side describes the normal elastic force based on Hooke’s law, and the last term is normal damping force using for energy dissipation.

Substituting all the force expressions from Eqs. (1) - (3), and Eqs. (8) - (14) in the force balance expression, Eq. (7) was solved numerically in three dimensions. The numerical solution of the ordinary differential equations of motion of the particles is based on an explicit integration procedure. The integration algorithm employed here is the half-step leapfrog Verlet scheme [14]. The discretization of particle velocity (Eqs. (15) - (16)) was carried out at each half time step while the trajectory equation (Eq. (17)) was discretised at each full time step and described as follows:
This numerical scheme indicates that the numerical integration of the acceleration term is performed twice over a time interval, $\Delta t$, to give the new velocity, and the new particle position equals the sum of the velocity at previous half time interval and the most recently obtained acceleration multiplied by the time step. A time step size of $\Delta t = 10$ ns was used in the DEM simulations. To check the accuracy of the model prediction, Schulze’s model on bubble-particle aggregate in quiescent liquid comprising Eqs. (1) - (4) were also solved using this integration algorithm. We refer the reader to Section 3.1 for more details.

3. Numerical modelling of single particle-bubble system

3.1. Algorithm comparison

In the following, we present a comparison between the MATLAB in-built multistep variable order Adams-Bashforth-Moulton PECE solver (ode113) and the DEM half-step leapfrog Verlet (HLV) scheme utilized in the numerical modelling with reference to the single particle-bubble interactions for interpreting the Schulze theory under quiescent conditions. A sketch detailing the particle-bubble system in two dimensions is given in Fig. 1(a).

Table 1. Input parameters for numerical simulations.

| Parameter                           | Value     |
|-------------------------------------|-----------|
| Particle radius ($\mu$m)            | 66        |
| Particle density (kg/m$^3$)         | 2500      |
| Bubble radius ($\mu$m)              | 900       |
| Water density ($kg/m^3$)            | 1000      |
| Water viscosity (Pa·s)              | 0.001     |
| Gas-water surface tension (N/m)     | 0.072     |
| Contact angle (°)                   | 70        |
| Initial radial position ($\mu$m)    | 400       |
| Initial polar position (°)          | 25        |

The results in terms of plot of particle radial position, $h$, versus time, $t$, is shown in Fig. 1(b). The tendency from this figure – not surprisingly – indicates that although the numerical methods differ, the comparison between the two types of simulation curves shows considerable similarities. For each case the particle was observed to fall at constant settling velocity (i.e. about 14 mm/s) as approaching the bubble, jump into contact with damped oscillation, and then finally reach a stable wetting perimeter. In an actual single particle-bubble system, the particle trajectory could deviate as a consequence of the hydrodynamic interaction due to the nearby boundary, that is, the bubble surface [8]. Additionally, the time for particle-bubble attachment to a large extend signifies the role of surface forces which should not be ignored. Finally, the magnitude of the jump-in distance is generally of the order of 10 μm [15] which is much smaller than the observed ~43 μm. As noted above the application of the Schulze theory to the simulation of particle-bubble interactions is not sufficient here, it is necessary that the hydrodynamic and surface chemistry aspects are taken into account. However, we analyze this force balance first because it is useful for developing the fundamental aspects of the calculation and analysis. We deal with a more realistic model of the system later using the 3-D DEM.
3.2. Comparison of complete DEM simulation with experimental results

Here, we compare our DEM modelling results with the experimental observations published previously in literature by Nguyen and Evans [16]. In their work, the system is the same as described in Section 3.1. The current DEM model has been further incorporated with hydrodynamic resistance functions, hydrophobic force and contact forces. The parameters can be found in both Table 1 and 2.

Table 2. Computation conditions used in the DEM simulations.

| Maximum hydrophobic force (μN) | Decay length (nm) | Restitution coefficient of particle-bubble contact (-) | Stiffness of particle-bubble contact (N/m) |
|-------------------------------|------------------|-------------------------------------------------------|----------------------------------------|
| 2                             | 15               | 0.2                                                   | ∞, 1, 0                                 |

For each individual simulation run, three different values of the particle-bubble contact stiffness were used: $k_{pb} = \infty$, 0 and 1 N/m. We first consider the cases where $k_{pb} = \infty$ and 0 N/m. Numerically, the former implies that the bubble is a perfectly rigid body leading to the situation where particle and bubble overlap may not be achieved. The latter is particular simple as the term $NCF$ in Eq. (7) vanishes.

The simulation results compared with the reported experimental data are shown in Fig. 2(a). In the experiment three distinct regimes of the particle motion around the bubble were found. In the first regime, i.e. from $t = 0$ to $t \approx 60$ ms, the particle radial position is observed to steadily decrease with time. When the particle came closed to the bubble surface, the hydrodynamics resistance effect became more conspicuous that the radial position remained almost unchanged during the following ~10 ms, which illustrated the second regime. The last regime describes the rupture of intervening liquid film accompanied by a jump-in distance of around 10 μm, and the expansion of TPCL to ultimately reach a maximum value. Regarding the first two regimes, the results are in qualitative agreement with the experimental observations, which is what would be expected. In other words, unlike the $h$-versus-$t$ curve illustrated in Fig. 1(b), the hydrodynamic resistance exhibited a significant role in the approaching of particle to the bubble surface at short separation distances, resulting in evident deviation of particle trajectory as well as decrease in particle speed. The discrepancy between simulation and experimental data in these regions might be ascribed to the hydrodynamic drag force model used in the DEM simulation, which is possibly diminished by using a more accurate force-displacement relationship. On the other hand, the properties of the particle and liquid in the physical experiment may not be accurately measured. It is important to note that, in the second regime, the hydrophobic force is found to have large influence on the film thinning and liquid drainage [17]. For example, when the decay length was reduced by an order of magnitude, that is, the particle surface has lower degree of hydrophobicity, the lifetime of the liquid film, therefore, will become longer. In contrast to the high similarities of these two cases (i.e. $k_{pb} = \infty$...
and 0 N/m) in the first two regimes, the particle in each case then behaved quite differently. As expected, we see from the green curve corresponding to $k_{pb} = \infty$ that the overlap of the particle and the bubble is closed to zero. When $k_{pb}$ becomes zero, which means that no information about the contact forces needs to be carried over from one time step to the next, the similar phenomenon – large jump-in distance observed in Fig. 1(b) will result. Therefore, the inclusion of bubble elasticity has a large effect on the particle-bubble attachment.

Next, we have fitted the parameter $k_{pb}$ to obtain exactly the same jump-in distance in the experiment of Nguyen and Evans. As shown in Fig. 2(b), in the case of $k_{pb} = 1$ N/m the simulation curve presents to be practically identical with the experimental one in the third regime, that is, both curves give ~10 μm of jump-in at the same time.

In summary, a comparison of experimental and DEM results on single particle behaviour around an air bubble surface test has demonstrated the potential of the proposed DEM simulations in the analysis of the particle-bubble interactions.

4. DEM simulation of interactions between attached particles

Under a real flotation environment, a rising bubble encounters clouds of particles which would interfere with each other’s movement, and possibly the particle-bubble aggregate stability. In this section we present predictions of interactions between two identical particles which are in contact with the bubble using the proposed DEM model.

A system has been selected whereby an air bubble (0.9 mm in radius) was stationary at the center of the working space, and one particle (labeled as Particle No. 1) was released far above the bubble, while the other (Particle No. 2) was positioned at the bottom at its equilibrium state of attachment with jump-in distance of ~30 μm. Both particles have radius of 200 μm, stiffness of particle-bubble contact of 1 N/m, stiffness of particle-particle contact of 1000 N/m, restitution coefficient of particle-particle contact of 0.74, and the other parameters are the same as presented in Table 1 and 2. Snapshots of the particle movement at different times are shown in Fig. 3. It can be seen in the images that the upper particle, Particle No. 1, gradually moved downwards under the action of gravity, followed by the collision and attachment to the bubble surface at $t$ is around 30 ms (see Fig. 4(a) Inset). Before the formation of a stable TPC we found, again, from Fig. 4(a) Inset that the particle radial position, $h$, fluctuated for a short time of about 10 ms after which the particle polar angle (see Fig. 4(b)) increased dramatically with time representing an enhancement in the particle sliding velocity. Two particles were in close proximity at about 64 ms, and then they collided and rebounded due to the large kinetic energy of Particle No. 1, resulting in two particles moving in opposite directions associated with slight fluctuations of $h$ but without the disengagement to the bubble. The second particle-particle encounter occurred at around 90 ms when the polar angles of two particles reached the peak, ~180° and ~200°, respectively (see Fig. 4(b)). Afterwards, both particles, as shown in Fig. 4(b), were sliding side by side rather than rebounding, rearranged and eventually rested at the underside of the bubble bringing the system a steady state.
It is notable that, in this scenario, particle size plays a significant role in the stability of particle-bubble aggregate. As particle size, thereby particle weight increases the momentum and kinetic energy before the particle-particle collision increases, leading to a more obvious and frequent rebound. Another factor influencing the particle movement is behind the DEM simulation algorithm, that is, the contact force-displacement relationship which is important for obtaining an accurate prediction of the strength of contact force as well as the frequency of collision. It must be emphasized that one might question the force-displacement relationship together with the parameters used here for evaluating the contact forces between spheres, however, we cannot provide convincing evidence because of the lack of published experimental data.

An interesting facet of this test is that we did not observe the particle-bubble detachment due to the strong capillary force. Indeed, particle properties, especially hydrophobicity, constitute the major part of the contribution to the particle-bubble aggregate stability, and thus the bubble loading capacity. In future work, we will focus on studying the interactions between different particles together with the investigation of the influences of particle properties including the size, the hydrophobicity, etc. on the particle-bubble aggregate stability.

Fig. 3. Particle movement around the bubble surface in snapshots.

Fig. 4. (a) Particle radial position and (b) polar angle as a function of time.
5. Conclusions

A DEM model for simulating particle-bubble interactions in quiescent liquids has been developed, tested and implemented. It has been shown from the simulation results that the motion of the particle around the bubble surface and the jump-in event can be accurately reproduced by adjusting the value of the elasticity of the bubble. Moreover, additional simulations for a sliding particle interacting with a stationary particle attached at the bottom of the bubble highlighted the collision and rebounding phenomena between particles. These findings prove the capacity of DEM simulation as a tool in the reliably studying the particle-bubble interactions. In this study, only the interaction behavior of identical spherical particles around the bubble was simulated, however the model is capable of simulating interactions of dissimilar particles (particles of different sizes and physical properties) which will be considered in future work.

Acknowledgements

Authors would like to thank Prof. Anh V. Nguyen for providing his experimental data. Guichao Wang would like to thank China Scholarship Council (CSC) for financial assistance.

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