Computational Study on the Effect of Particle Shape on Particle-Bubble Interactions Using Discrete Element Method

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Abstract

Utilizing particle-bubble mechanics theory, we developed a three-dimensional Discrete Element Method (DEM) model to simulate interactions between particles and bubbles. Six distinct irregular particle geometries were incorporated. Simulations examined both spherical and irregularly shaped diaspore particles (0.1 mm, surface-modified) with contact angles of 35.6°, 55.4°, and 85.7° interacting with a stationary bubble in quiescent water. Results indicate a five-stage interaction process for both particle types: free settling, bubble surface flow, liquid film sliding, film rupture and three-phase contact line (TPCL) formation, and TPCL sliding. Compared to spheres, irregular particles exhibited a larger critical collision angle and higher capture probability, alongside a shorter critical induction time. Their edges and vertices facilitate liquid film thinning and rupture between the particle and bubble, thereby reducing induction time and enhancing capture probability.

Keywords: Discrete Element Method, Particle-bubble interaction, Particle shape, Critical collision angle, Critical induction time.

1. Introduction

Flotation is an efficient method for separating fine minerals, which is to achieve selective separation of useful minerals and gangue minerals according to the differences in the physical and chemical properties of the surface of mineral particles [1, 2]. As the basic action unit of the flotation process, the particle-bubble interaction determines the flotation efficiency to a certain extent, which can be divided into three sub-processes: the particle-bubble collision, the particle-bubble attachment, and the particle-bubble detachment. Particle shape characteristics play a crucial role in these sub-processes [3]. Particle shape remarkably affects the induction time and flotation recovery. Induction time is the time interval between the initial contact of the particle and bubble and the formation of a stable three-phase contact line. Verrelli et al. [4, 5] studied the variation of the induction time between spherical and irregular particles at different approach speeds, and the results showed that the induction time between irregular particles and a bubble was an order of magnitude lower than that of spherical particles, and the induction time decreased with the increase of approach speed. Hassas et al. [6] found that irregular surface bulges and sharp edges can effectively trigger the rupture of liquid film and improve the flotation recovery. Wen and Xia [7] found that the low-ash anthracite particles with lower roundness can be floated quickly, while the low-ash anthracite particles with higher roundness floated slowly. Ulusoy [8, 9] states that the study found that particles with higher elongation and less roundness had higher flotation recovery than particles with lower elongation and higher roundness. It is generally believed that the protrusions and sharp edge structures on the surface of irregular particles contribute to the rapid thinning and rupture of the particle-bubble liquid film [10]. Therefore, irregularly shaped mineral particles usually have higher flotation recovery and flotation rate compared with spherical particles.

However, the effect of particle shape on particle-bubble interactions is difficult to evaluate for the following reasons. First, the particle size of flotation particles is small. It is difficult to describe the three-dimensional shape of the particles, and there is no accepted method to characterize the three-dimensional shape of the flotation particles accurately [11]. Secondly, when preparing particles of various shapes, the surface roughness of the particles also changes [12]. For the above two reasons, it is a great challenge to experimentally study the effect of particle shape on the behavior of particle-bubble interactions.

In recent years, the Discrete Element Method (DEM) was successfully used in simulation to study the particle-bubble interaction problem in flotation. Maxwell et al. [13] developed a DEM model of particle-bubble interaction. They computationally analyzed the effect of particle size distribution and hydrophobic force on particle-bubble collision and particle sliding on the bubble's surface. Moreno-Atanasio [14] compared and studied the effects of different Hydrophobic force models (power decay law and single exponential law) on bubble capturing particles. Gao et al. [15] studied the effect of hydrophobic forces on particle-bubble interactions using a single exponential decay type formula for hydrophobic forces. It is found that when the decay length λ is less than 10 nm, the number of particles captured by the bubbles is independent of the strength of the hydrophobic force, and when λ is in the range of 10-500 nm, the capturing efficiency increases significantly with the strength of the hydrophobic force and λ. In subsequent work, Gao et al. [16] performed DEM modeling based on the Schulze particle-bubble aggregate theory [17] to simulate the sliding of particles on the surface of the bubble and the formation of a TPCL. However, none of these works based on DEM to simulate particle-bubble interactions have considered the effect of particle shape on particle-bubble interactions.

This work presents a 3D computational model of particle-bubble interactions based on the Discrete Element Method (DEM) in quiescent liquid and designs six models of irregularly shaped particles. Spherical particles were used as a control group, and the effects of particle shape on the behavior of particle-bubble interactions, critical collision angle, and capture probability were investigated. Furthermore, the single irregular particle bubble interaction behavior was compared with the reported experimental data to verify the accuracy of the simulation.

2. Simulation Methodology

2.1 Model Description

The three-dimensional schematic diagram of the simulation system is shown in Figure 1. The bubble was fixed at the coordinate origin O in a quiescent water environment. The particles are generated and released in turn along the positive direction of the X-axis on the horizontal plane $3R_b$ (R_b = bubble radius) above the bubble center O. In other words, each particle generation position is a certain distance more in the positive direction of the X-axis than the last particle generation position. The positions where the particle is generated are cycled in this way until the particle is released at a specific position on the X-axis, and the bubble cannot capture the particle. In this simulation, the position where the particle velocity reaches the minimum value during the process of a particle approaching the bubble was set as the collision point. The angle between the line connecting the center of the bubble and the collision point and the positive direction of the Z-axis was defined as the collision angle (φ).

particles of the same contact angle. It is indicated that the effect of particle shape on the critical induction time increases as the hydrophobicity of the particles decreases.

All these prove that the critical induction time of irregular particles is smaller than that of spherical particles. In other words, irregular particles' sharp and edge shapes can promote the thinning and rupturing of the liquid film between particles and bubbles during the particle-bubble interaction, thereby shortening the induction time.

To sum up, in the process of particle-bubble interaction, owing to the surface of irregular shape particles having sharp edge shapes, it is easier for irregular shape particles to rupture the liquid film between particle and bubble than spherical particles, which have the advantage of shortening the attachment time and improving the attachment probability and then improving the capture probability of bubble to irregular shape particle.

4. Conclusions

In this work, six irregular particle models with different shapes are designed. The interaction behavior of spherical particles and irregularly shaped (a-f) particles and a bubble was simulated by DEM. The effect of particle shape on particle-bubble interaction behavior, critical collision angle, capture probability, and critical induction time was investigated. The principal findings of the study are summarized below:

1. Spherical and irregularly shaped particles can be divided into five stages during their interaction with the bubble: (1) Free settling (2) Flow around the bubble surface (3) Sliding with a liquid film (4) Film rupture and TPCL formation (5) Sliding with a TPCL. However, compared with spherical particles, in film rupture and TPCL formation stage, the edges and corners of irregular particles first contact with a bubble to form TPCL, resulting in particle imbalance and rotation.
2. Irregular shape particles have the advantage of a larger critical collision angle and capture probability than spherical particles. This advantage increases with decreasing particle sphericity and enhances with decreasing particle hydrophobicity.
3. Irregular particles have a smaller critical induction time than spherical particles. Irregular particles with edges and corners can promote the thinning and rupture of the liquid film between bubble and particle.

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