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Sticking/rebound criterion for collisions of small adhesive particles: Effects of impact parameter and particle size

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ABSTRACT

The collision-sticking phenomenon among micron-sized particles is ubiquitous in nature and plays an important role in formation of particle agglomerates or deposits. In this paper, a validated 3D JKR-based discrete-element method (DEM) is employed to investigate oblique collisions of micron-sized particles. Special attention is paid to the effects of impact parameter and particle size on the sticking/rebound criterion and energy dissipation pathways. Various energy dissipation mechanisms, including viscoelastic effect, sliding resistance and rolling resistance, are incorporated in our DEM model. Based on our simulation results, the temporal evolution for the collision process is revealed in detail to establish a deeper understanding of collision dynamics. Moreover, two regimes are clarified according to the effect of impact angles on the sticking criterion. In the low impact angle regime, the normal critical velocity V_{CN} keeps as a constant. While in the regime of high impact angle, V_{CN} rapidly drops. Furthermore, the strong effect of particle size ratio on the critical velocity is also analyzed. This effect can be well described by the dimensionless adhesion parameter, *Ad*. Finally, a generalized formula is drawn as the sticking/rebound criterion for collisions of fine particles, which can be readily implemented in computational fluid dynamics (CFD) codes.

1. Introduction

Collision and coagulation of micron particles, existing in a variety of areas of engineering, biology, astrophysics and environmental science, play a central role in determining the structure of particle agglomerates or deposits [1–4]. The question whether or not a collision may result in sticking is of importance for the evolution of agglomerates [5,6]. In the size range of 10 microns or smaller, the van der Waals force between particles is more significant than the gravitational force or fluid force and is primarily responsible for holding the dust particles together [7]. The interaction between colliding particles becomes quite complicated due to the presence of the adhesive force.

In order to describe coagulation processes properly, a physical understanding of binary collisions is prerequisite. During the collision process with adhesion taken into account, relative motions (e.g., normal overlapping, relative sliding, rolling and twisting) between contact particles take place accompanied by diverse energy-loss mechanisms including internal friction, viscoelastic response, interfacial slip, etc [8–11]. Owing to the adhesion force between contact particles, a gentle collision with an impact velocity less than the critical sticking velocity V_C will result in sticking. And both the viscoelastic damping force and the adhesive force contribute to the energy loss [12,13]. On the other hand, colliding particles will bounce off each other when collision velocities exceed V_C. By introducing the coefficient of restitution *e*, defined as the ratio of the relative post- and pre-collision velocities, the outcome of an energy-dissipated bouncing collision can be quantitatively described.

Various experimental and theoretical studies have been published over the decades on the critical sticking velocity V_C and the coefficient of restitution *e* [14–17]. Among those experimental studies, one of the most extensive data for normal collisions between micron particles and a surface is from Wall et al. [16]. Güttler et al. provided an overview on published literatures describing experiments on normal collisions, with a focus on the relationship between the coefficient of restitution and the incident velocity [18]. However, due to the small size of micron particles and the ultra-short time scale associated with particle collisions, the inability to observe the detailed information and the failure to account for tangential or rotational velocities during collision experiments have greatly limited the physical understanding of the processes. From the theoretical level, simplified analytical solutions for the critical sticking velocities were proposed by both Dominik and Tielens [2] and Thornton and Ning [17]. However, only the energy required to separate contact surfaces was considered in their simplified models, and the interaction between particles was considered to be elastic, which is inconsistent with the practical situation. In a real collision, many factors, including the viscoelasticity of materials, the collision angles and the

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size of particle, contribute to the sticking criterion. Therefore, it's hard to predict V_C with a single formula.

To better understand these collision problems, it is essential to propose an appropriate micro-dynamic model describing the interactions between contact micron particles. Dynamic models generally describe the impact process through a combination of quasi-static contact theories and dissipation mechanisms [1,7,19]. The theory on quasi-static contact usually serves as a fundamental description of the contact, while energy dissipation mechanisms account for the dynamic effects such as viscoelasticity of materials. A variety of models exist to describe the effect of van der Waals adhesion on the elastic force during static contact of particles. Among these models, the JKR (Johnson, Kendall and Roberts), DMT (Derjaguin, Muller and Toporov) and M-D (Maugis-Dugdale) models are widely accepted and applied for regimes with different Tabor parameter λ_T [20–22]. The JKR model assumes that the adhesive force acts only inside the contact region [20] and is appropriate for relatively large, compliant particles for which the Tabor parameter λ_T is large compared to unity [1]. Based on the JKR model, the dynamic process of normal impacts between micron particles and a flat surface was described by Liu et al. and the results have been validated by classic particle/surface impact experiments [12,16]. Liu et al. also concluded that the JKR model can give proper predictions of contact size and overlap even in conditions beyond the expected JKR range [23]. Recently energy dissipated in head-on collisions between two spheres was further investigated by Krijt et al. [13], in which a collision model with combined energy-loss mechanisms including adhesion, viscoelasticity and plastic deformation was presented.

However, aforementioned studies mostly focused on *normal* collisions between particles or between a particle and a surface. Generally, the collisions between two spheres are oblique with non-zero impact angles which may give rise to a highly coupled inter-particles motions including normal overlapping, sliding and rolling. The notion of normal critical velocity V_{CN} has been exploited as a sticking/rebound criterion without consideration of the effect of rolling and sliding motions in the tangential degree. Thus, this simplistic criterion has a serious limitation for collisions with high impact angle θ. Konstandopoulos found that, when the impact angle is larger than a critical value, the sticking cannot happen despite that $V_N < V_{CN}$ is met [24]. A three-dimensional simulation has also shown that the approach of energy conversion due to tangential motions is quite sensitive to the impact angle and will affect the outcome of a collision [25]. Despite the efforts made to model tangential friction problems caused by oblique collision [10,11,26], an explicit expression of the sticking criterion V_{CN}, which is of great importance for incorporation into CFD codes or simulations describing particle deposition and coagulation processes, is really needed but still not drawn out yet.

More recently, Li and Marshall [27], and Marshall [28] developed a three-dimensional discrete-element method for adhesive micron-sized particles based on the JKR model (termed as adhesive DEM hereinafter), and successfully applied it to dynamic simulations of microparticle deposition on both flat and cylindrical surfaces with a series of experimental validations [7,29]. By using this adhesive DEM approach, not only macroscopic parameters (e.g., the restitution coefficient and the critical sticking velocity) can be predicted, but also microscopic information (e.g. the contact area, the normal overlapping and the relative sliding distance) during a collision can be provided. This DEM approach enables us to further explore a generalized expression for the sticking/rebound criterion of collisions covering all impact angles.

In addition, changing of particle size will lead to a variation of relative importance of particle inertia and adhesive force. With particles' size increasing from micrometer to millimeter or even larger, a transition from adhesion-dominant regime to inertia-dominant regime will give rise to quite different results of collisions [30]. Fractions of energy dissipated due to various mechanisms also change with the particle size. And this significant size-effect on the outcome of a collision can also be investigated by the adhesive DEM.

In this paper, we focus on oblique collisions between micron particles by employing a three-dimensional adhesive DEM. The central issue addressed in this paper is whether particles of a certain size will stick or not upon collisions with a given impact parameter and how the kinetic energy of colliding particles is dissipated. The structure of the paper is as follows: the brief introduction of adhesive DEM, including the JKR-based models together with various energy dissipation mechanisms, is given in Section 2.1 and Section 2.2; then the collision geometry is given in Section 2.3; and the results and discussion, including microscopic information of oblique collisions and the effects of impact parameter and particle size on the sticking criterion are presented in Section 3.

2. Models and method

2.1. Adhesive DEM

The current investigation involves simulations of inter-particle collisions by employing a three-dimensional DEM approach for adhesive particles. In this adhesive DEM, particles are regarded as soft spheres whose momentum and angular momentum equations are solved by incorporating various models to describe the contact force, for an overview see, e.g. [1,7,27]. In this work, only adhesive contact forces $\mathbf{F}_A$ and torques $\mathbf{M}_A$ during particle collision are taken into account. The JKR model was employed to describe the elastic contact force F_{ne} as a combination of adhesion and elastic deformation of particles. The expressions for F_{ne} and normal overlap δ_N are written in terms of the contact region radius $a(t)$ [1],

$$\frac{F_{ne}}{F_C} = 4\left(\frac{a}{a_0}\right)^3 - 4\left(\frac{a}{a_0}\right)^{3/2}, \quad \frac{\delta_N}{\delta_C} = 6^{1/3}\left[2\left(\frac{a}{a_0}\right)^2 - \frac{4}{3}\left(\frac{a}{a_0}\right)^{1/2}\right], \tag{1}$$

where the critical force and overlap, F_C and δ_C, and the equilibrium radius, a_0 are given by

$$F_C = 3\pi\gamma R, \quad \delta_C = \frac{a_0^2}{2(6)^{1/3}R}, \quad a_0 = \left(\frac{9\pi\gamma R^2}{E}\right)^{1/3} \tag{2}$$

which are all expressed in terms of effective parameters, including the particle radius $R = (r_i^{-1} + r_j^{-1})^{-1}$, the elastic moduli $E = ((1-\nu_i^2)/E_i + (1-\nu_j^2)/E_j)^{-1}$, the shear moduli $G = ((2-\nu_i)/G_i + (2-\nu_j)/G_j)^{-1}$ and the surface energy $\gamma = \sqrt{\gamma_1\gamma_2}$.

Apart from the JKR elastic contact force, we consider the viscoelasticity of materials. The solid-phase dissipation force is assumed to be proportional to the rate of change of the material deformation in the form

$$F_{nd} = \eta_N \mathbf{v}_R \cdot \mathbf{n} = \eta_N \frac{d\delta_N}{dt}. \tag{3}$$

Here, the normal dissipation coefficient $\eta_N = \alpha(m^* k_N)^{1/2}$ is described in literature [9] and $\mathbf{v}_R = (\mathbf{v}_i + \mathbf{\Omega} \times \mathbf{r}_i) - (\mathbf{v}_j + \mathbf{\Omega} \times \mathbf{r}_j)$ is the relative velocity at the contact point on particle surfaces. For head-on collisions between two bulk particles with negligible adhesion or plastic deformation, the viscoelasticity effect is the only dominant factor to dissipate energy and the restitution coefficient is almost kept in a fixed value, e_0, which is related to the damping coefficient α. Both e_0 and α can intrinsically reflect the damping properties of adhesionless particles, with their relationship studied in literatures [1,28]. However, as for collisions between micron-sized particles in presence of adhesion, both inter-particle adhesion and the damping properties affect the outcome of the collision [12–14]. As a result, the restitution coefficient e ranges from 0 for sticking collisions to e_0 for inertia-dominant collisions. Here, we set the surface energy $\gamma = 15$ mJ/m^2 and the coefficient $e_0 = 0.6$ to account for the damping effect. Then a sixth-order formula $\alpha =$