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Mechanistic studies of initial deposition of fine adhesive particles on a fiber using discrete-element methods ☆

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ABSTRACT

The impaction-sticking mechanism of fine particulates plays a significant role in a wide range of applications from dust separation devices, thin-film deposition techniques to the astrophysics science, but the underlying physics still remains unclear. In this paper, a discrete element method (DEM) approach is established to investigate the impaction-sticking process during the initial deposition of fine particles on a single fiber. Starting from the JKR adhesive contact theory, the DEM well predicts the measured trend of single-fiber capture efficiency as a function of Stokes number in the literature, by the proper considerations of key dissipation terms including the first-contact energy loss, the linear-dashpot damping and the rolling friction resistance. The increasing work of adhesion not only dramatically increases the peak value of single fiber efficiency, but also causes the peak to move towards a much higher Stokes number. The DEM predictions further clarify that the sticking probability depends on the adhesion parameter, rather than Stokes number. An empirical power law between sticking probability and adhesion parameter is drawn as $h = 0.0558 \cdot \mathrm{Ad}^{5/3}$ (for $\mathrm{Ad} < 5.65$). Finally, by using both adhesion parameter for the sticking and Stokes number for the impaction, four distinct deposition patterns during the initial stage of single fiber filtration are identified.

1. Introduction

The underlying physics of the deposition and removal of fine particulates in various fields of air pollution, microelectronics and pharmaceutical industries are of both interest and importance. The flow behavior of fine particulates differs greatly from that of larger, non-adhesive granular materials that are governed mostly by gravitational, collisional and frictional forces [1,2]. For instance, the attractive forces between the particles of micron or sub-micron sizes are substantially higher than the gravitational or inertial forces, which cause fine particles to adhere upon collision and form agglomerates. Among all kinds of intermolecular adhesions, the dispersive adhesion due to van der Waals attraction of molecules in the contact zone of binary particles plays a central role, particularly for neutral small particles, since the adhesion always exists and becomes dramatically important when two particles approach to a short range [3].

Discrete element modeling (DEM), one of Lagrangian particle methods mainly for describing big granular materials, has received a renewed attention to fine particles [2,4–8]. DEM can directly consider particle adhesion and collision at a microscopic grain level while other approaches, such as two-fluid models, Brownian or Stokesian dynamics, cannot handle the problem. Li, Marshall and co-workers pointed out that the existence of van der Waals adhesion introduces a range of difficulties for the simulation of particle behavior in particulate flows [2,4]. First, there is wide diversity between the ultra-short time scales associated with particle adhesion/collision and the much longer time scales associated with fluid motion, which causes a stiff numerical solution of particulate flows. Second, the presence of adhesion introduces the necessity of modeling not only the adhesive force itself, but also the effect of adhesion on various particle contact forces. Hence, in order to develop a DEM for fine particles, the selection of a proper adhesive contact model is important. There are two classic adhesion contact models, the JKR (Johnson, Kendall and Roberts) theory assuming the adhesive force acting inside the contact radius, and the DMT (Derjaguin, Muller and Toporov) theory assuming the adhesive force acting outside the contact area [9,10]. More recently, Liu et al. discussed the applicability of different adhesion models for their use in DEM of fine particulate flows, and concluded that, for particles at micro-sizes, JKR equations give good predictions of the contact size and overlap even in conditions beyond the expected JKR range [11].

Extending a quasi-static JKR theory for a generalized DEM framework of fine adhesive particles has encountered the following challenges. First, in dynamic normal collisions between two particles or a particle and the wall, the energy dissipation accounting for dynamic effects such as viscoelasticity of materials must be incorporated into the JKR adhesive-elastic model. On the basis of normal pressure distribution over contact area predicted by the JKR theory, Thornton

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and Ning proposed the cut-off corresponding to a limiting contact pressure p_y for the plastic deformation, known as the adhesive elastic–plastic model [12]. However, the complexity of the equations inhibits its application in the DEM simulation of adhesive spheres. Hence several damping force models, e.g., a simple linear-dashpot to the overall JKR normal forces and a two-component linear dashpot to both the attractive and repulsive components of JKR forces, were successfully developed [2,13]. These simple JKR-based damping models were validated by classic particle/surface impact experiments in the aerosol community [14,15], in which both the coefficient of restitution and the critical sticking velocity of bouncing particles are well predicted [2,13]. Second, different to densely-packed granular materials, fine particles naturally form low-density agglomerates mainly consisting of quasi-linear dendrite-like chains [16,17]. It can be attributed to the rolling resistance of JKR contact, which is related to the asymmetry in the contact region induced by the van der Waals adhesion. An approximate torque model proportional to the rolling displacement was proposed by Dominik and Tielens and then validated by AFM experiments [18,19]. As for other frictional mechanisms, Thornton and co-workers considered the effect of van der Waals adhesion on the tangential sliding force and proposed a relatively simple model [20,21]. Comparatively, the sliding is relatively rare for fine particles due to the small momentum, and it is of importance mainly in cases where an aggregate is torn apart by a fluid shear or by adhesion to another aggregate [4]. Finally, the multi-time scale computational approach was introduced for solving the aforementioned wide diversity between various particle and fluid time scales. The DEM framework of adhesive particulate flows has be successfully established and developed [2,4].

A single-fiber (SF) capture experiment, namely the collection of small particles on an individual fiber, was intensively used as a *prototypical system* for clarifying fundamental physics of particle deposition or agglomeration [22,23]. In addition, the SF capture is an essential element of understanding complex fibrous filtrations that are widely employed in power, mining and cement industries as well as life and work areas. One of the most important macroscopic parameters for the system is the capture efficiency, η, of single fiber. Generally, the SF efficiency η can be decoupled as the product of the collision efficiency of particles to a fiber (φ) and the sticking probability (h) upon the impaction [24]. The former relates to the particle motions in main fluids and boundary layers, while the latter is balanced by the inertia of incident particles and the adhesion work between particles or a particle and the wall. Within past decades, dozens of literatures reported the studies on the collision efficiency by using both experiments and CFD simulations, in which several empirical expressions were drawn to relate φ to the Stokes number ($\mathrm{St}\equiv\rho_p d_p^2 U_0/18\mu L$) and Reynolds number ($\mathrm{Re}_F\equiv\rho_f U_0 L/\mu$) [25–27].

Comparatively, the studies on sticking probability, also named as adhesion efficiency, are much less. Hiller and Löffler derived a semi-empirical expression for the sticking probability based on theoretical considerations for the collision and energy loss of particles interacting with the fiber in a validity range of $\mathrm{Re}_F<1$ and $1<\mathrm{St}<20$ [26]. Ptak and Jaroszcyk later obtained a new fitting function based on the measurements with dust particles in actual filter media for a much wider $\mathrm{Re}_F<6$ [27]. More recently, Kasper et al. used monodisperse polystyrene aerosols (1.3, 2.6, 3.6 and 5.2 μm) to precisely measure the single fiber efficiency data for the inertia-interception regime of both bare fibers and dust loaded fibers [24]. As for the initial deposition stage of a bare fiber, the remarkable discrepancy between the experimental data and the existing analytical model [26,27] at higher *St* implies that the physical mechanisms of sticking probability need to be further clarified.

Previous computational approaches on the deposition of fine particles on a single fiber focused on the trajectory analysis [28,29] and incident particle kinetic model [30,31]. All of these models, different to dynamic model, assume that once a particle is determined to be "stuck" to the fiber or to the aggregate surrounding the fiber, it is frozen in place. This assumption conflicts with the existing experimental observations as well as empirical formulas of sticking probability [5,24]. Comparatively, the aforementioned DEM based on JKR theory, that can simulate intrinsic contact dynamics at microscopic grain level, is intriguing to be employed to investigate the sticking/rebound probability of particles on the single fiber and to draw the dimensionless criteria governing the adhesion efficiency.

In this paper, we employ a JKR-based DEM approach to intensively study the mechanisms of initial deposition of fine particles on a single fiber. Section 2.1 briefly introduces DEM framework, the JKR theory and dissipation models such as plastic damping and rolling, twisting and sliding frictions. Then the simulated system and computational details are given in Section 2.2. Finally, the results and discussion are performed in Section 3, in which the dependence of SF efficiency, the dynamics of particle sticking/rebound, the determination of sticking probability and its governing factors, and the distinct initial deposition patterns of SF capture are particularly focused on.

2. Models and method

2.1. Description of DEM approach

In the DEM approach, the transitional and rotational motions of each particle are expressed by Newton's second law of motion,

$$m\frac{d\mathbf{v}}{dt} = \mathbf{F}_F + \mathbf{F}_A, \quad I\frac{d\mathbf{\Omega}}{dt} = \mathbf{M}_F + \mathbf{M}_A, \tag{1}$$

where $\mathbf{v}$ and $\mathbf{\Omega}$ are respectively the centroid velocity and rotation rate of an arbitrary particle, m is the particle mass, $I=(1/10)md_p^2$ is the moment of inertia, and dp is the particle diameter. $\mathbf{F}_F$ and $\mathbf{M}_F$ are the fluid force and torque on this particle in the viscous regime, while the sum of all adhesive contact forces $\mathbf{F}_A$ and torques $\mathbf{M}_A$ acting on a particle can be expressed for the collision of two spherical particles as,

$$\mathbf{F}_A = F_n\mathbf{n} + F_s\mathbf{t}_S, \quad \mathbf{M}_A = r_iF_s(\mathbf{n}\times\mathbf{t}_S) + M_r(\mathbf{t}_R\times\mathbf{n}) + M_t\mathbf{n}, \tag{2}$$

where $\mathbf{n}$ is the unit normal vector along the line passing through the particle centroids. Here F_n is the magnitude of the normal force acting along $\mathbf{n}$. F_s is the magnitude of the sliding resistance, and this tangential force acts in a direction $\mathbf{t}_S$ corresponding to the direction of the relative motion of particle surfaces at the contact point, projected onto the plane and orthogonal to $\mathbf{n}$. The tangential force results in a torque of $\mathbf{M}_S=r_iF_s(\mathbf{n}\times\mathbf{t}_S)$. The twisting resistance exerts a torque on the particle oriented normal to the contact plane. Particularly, an important side-effect of van der Waals adhesion is the introduction of a rolling resistance [2,4,18], which exerts a torque on the particle in the $\mathbf{t}_R\times\mathbf{n}$ direction, where $\mathbf{t}_R$ is the direction of the "rolling" velocity.

As for particle–particle interactions, we consider two particles with radii r_i and r_j, elastic moduli E_i and E_j, Poisson ratios ν_i and ν_j, shear moduli $G_i=E_i/2(1+\nu_i)$ and $G_j=E_j/2(1+\nu_j)$, and surface energies γ_i and γ_j. An effective particle radius, R, and elastic and shear moduli, E and G, and the work of adhesion, $W=2\gamma$, are defined by

$$\frac{1}{R}\equiv\frac{1}{r_i}+\frac{1}{r_j}, \quad \frac{1}{E}\equiv\frac{1-\nu_i^2}{E_i}+\frac{1-\nu_j^2}{E_j}, \quad \frac{1}{G}\equiv\frac{2-\nu_i}{G_i}+\frac{2-\nu_j}{G_j}, \quad W=2\gamma=2\sqrt{\gamma_1\gamma_2}. \tag{3}$$

Table 1 summarizes the expressions for all related adhesive contact forces and torques as well as their calculating coefficients. The JKR theory is used for the normal elastic contact force F_{ne}. In order to simplify construction of a DEM simulation, a non-dimensional Chokshi expression, rearranging JKR theory to express F_{ne} in terms of the contact region radius $a(t)$ and the normal overlap δ_N, is introduced here [32]. The dissipation due to first-contact loss is