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Simulation of entrainment of agglomerates from plate surfaces by shear flows

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ABSTRACT

The entrainment process of agglomerates deposited on plate surfaces by shear flows was simulated using the three-dimensional modified discrete element method (mDEM) and influences of several factors on entrainment process were examined. In the case shear induced force is too weak, deposits are only deformed and particles are barely entrained, however, above some critical value particles are entrained by flows forming agglomerates. It was also clarified that the steric-bulky deposit undergoes the stronger hydrodynamic force and is easy to be entrained. There are two entrainment mechanisms corresponding to the parameter A_s/A which indicates the relative strength of adhesive force between particle and plate surface to that between particles. In case of large A_s/A where the adhesion between particle and plate surface is predominant, the number of entrained particles monotonically decreases as A_s/A increases due to the enhanced binding force. By contrast for small A_s/A, the number of entrained particles is not heavily dependent on A_s/A due to the mechanism in which the upstream side of deposit is lifted and the deposit is deformed extensively then large agglomerates are entrained. The boundary between those two entrainment mechanisms exists at $A_s/A = 0.5-0.6$ which is in good agreement with the theoretical prediction.

1. Introduction

Small particles adhere to surfaces through various interactions such as van der Waals attraction and electrical interaction. The detachment of these particles from plate surfaces is important for many industrial processes such as silicon wafer cleaning process. In such a process, removal of foreign contaminant particles is a critical technology to determine the product yield. Usually such a detachment is done by applying gas or liquid jets and particles are entrained by the hydrodynamic force imposed by the fluid media. Therefore it is important to know the entrainment mechanism and microscopic behavior of deposits as well as hydrodynamic interaction between particles and fluids. Many researchers have investigated and reported entrainment of fine particles from surfaces using gas jet flows theoretically and experimentally (Corn and Stein, 1965; Zinkend et al., 1995; Otani et al., 1995; Masuda et al., 1994; Smedley et al., 1999). Both the normal lift force and the tangential shear force have been proposed as the impetus for detachment of particles. Phares et al. (2000) did an intensive investigation including laminar flow regime and reported the threshold shear stress data as well as comparison with theories. Although liquid jet is a potential method of stronger hydrodynamic force, unfortunately the entrainment of particles in liquid phase has not been reported so far.

The previous works have focused on the entrainment of relatively large (ca 8–20 μm in diameter) non-agglomerated particles, although it is well known that fine particles are colloidally unstable and easy to coagulate (Russel et al., 1989; Hunter, 1987). Hence it is plausible to consider contaminant particles are deposited on a surface forming agglomerates and the coagulation of particles should definitely alter the nature of entrainment. However, there is no report on the entrainment of agglomerates instead of its extreme importance. One reason for this is that the phenomenon occurs within an extremely short period of time and small space as well as its excessive complexity, and thus the experimental approach has limitations. Computer simulation might be a potentially powerful tool to investigate the phenomenon. Recently several simulation methods such as Stokesian dynamics (Harada et al., 2006) and lattice Boltzmann method (LBM) (Inamuro and Ii, 2006) have been applied to the simulation of agglomerate behavior in flows. Although they are accurate numerical models, computational load is high and they are applicable to only simple systems. In our previous works modified discrete element method (mDEM), in which hydrodynamic interaction between particle and fluid and local porosity of agglomerates are taken into account, has been developed and proven to be versatile and effective to simulate the behavior of agglomerate such as breakup in flows (Higashitani et al., 2001; Iimura et al., 1998; Iimura and Higashitani, 2005).

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In this work mDEM is applied to simulate the entrainment process of deposits composed of agglomerated particles from a flat plate surface by shear flows in liquid phase. The influences of deposit structure, magnitude of flows and interaction between particle and plate surface are investigated and reported.

2. Model

The detail of mDEM model has been reported in our previous publications (Higashitani et al., 2001; Iimura et al., 1998; Iimura and Higashitani, 2005), here it is summarized only briefly. And the definition of interaction between particle and plate surface as well as the evaluation method of entrainment is described.

2.1. mDEM model

Consider an arbitrary shaped agglomerate which is composed of N spherical mono-dispersed particles of radius a and of density ρ_{p}. By integrating equations of motion for translational and rotational motions expressed by Eqs. (1) and (2), the velocity as well as position and angular velocity of each particle can be obtained when total force $\boldsymbol{F}_i$ and torque $\boldsymbol{T}_i$ on the objective particle are given:

$$m\frac{\mathrm{d}\boldsymbol{v}_i}{\mathrm{d}t} = \boldsymbol{F}_i \tag{1}$$

$$I\frac{\mathrm{d}\omega_i}{\mathrm{d}t} = \boldsymbol{T}_i \tag{2}$$

where t is time, m $(=\rho_{\mathrm{p}}\frac{4}{3}\pi a^3)$ and I $(=\rho_{\mathrm{p}}\frac{8}{15}\pi a^5)$ are the mass and moment of inertial of a constituent particle, respectively, $\boldsymbol{v}_i$ and $\boldsymbol{\omega}_i$are the velocity and angular velocity of particle i. Verlet algorithm was employed as integration algorithm. Total force and torque are the sum of the hydrodynamic and inter-particle contributions as well as gravitational force thus expressed as following:

$$\boldsymbol{F}_i = \boldsymbol{F}_{\mathrm{h}i} + \sum_j \boldsymbol{F}_{\mathrm{p}ij} + (\rho_{\mathrm{p}} - \rho_{\mathrm{f}})\frac{4}{3}\pi a^3 \mathbf{g} \tag{3}$$

$$\boldsymbol{T}_i = \boldsymbol{T}_{\mathrm{h}i} - \frac{1}{2}\sum_j \boldsymbol{r}_{ij} \times \boldsymbol{F}_{\mathrm{p}ij} \tag{4}$$

where ρ_{f} is density of the fluid, subscript h indicates the hydrodynamic contribution, $\boldsymbol{F}_{\mathrm{p}ij}$ is the force exerted on particle i by particle j and $\boldsymbol{r}_{ij}$ is the relative position vector of particle i to particle j.

In mDEM model, two kinds of interactions between particles are considered. When two particles are not in contact, they are assumed to interact with each other through the van der Waals attractive force. By contrast when two particles are in contact due to the trial displacement of DEM algorithm, a repulsive contact force is assumed to act between them because of the volume exclusion effect. The van der Waals potential $V_{\mathrm{A}ij}$ between two spherical particles i and j of identical size is a function of distance which is given by the following equation (Russel et al., 1989; Verway and Overbeek, 1948; Dzyaloshinskii et al., 1961; Mahanty and Ninham, 1976; Israelachvili, 1991):

$$V_{\mathrm{A}ij} = -\frac{A}{6}\left(\frac{2a^2}{r_{ij}^2 - 4a^2} + \frac{2a^2}{r_{ij}^2} + \ln\frac{r_{ij}^2 - 4a^2}{r_{ij}^2}\right) \quad (\text{for } r_{ij} \geqslant \delta_{\min}) \tag{5}$$

where A is the Hamaker constant. The minimum separation between two particle surfaces $\delta_{\min}$ is assumed to be 4 Å for clean flat surfaces (Krupp, 1967). The corresponding attractive force is given by $-\mathrm{d}V_{\mathrm{A}ij}/\mathrm{d}r_{ij}$.

When the distance between particle is smaller than $\delta_{\min}$, the repulsive contact force can be calculated using conventional DEM algorithm which was first developed by Cundall and Struck (1979) and has been reported by a large number of successors elsewhere (Tsuji et al., 1993; Di Renzo and Di Maio, 2004). Normal and tangential contact forces can be obtained assuming the Voigt elements in both directions as shown in Fig. 1. The spring constant in normal direction K^{n} was assumed to be 100 N/m empirically in consideration of the stability of calculation. The other values were calculated according to the conventional way (Cundall and Struck, 1979; Tsuji et al., 1993), K^{t} was given by $K^{\mathrm{n}}/10$ and the decay constant of dashpot η for both directions could be calculated by the following equation as a function of spring constant K:

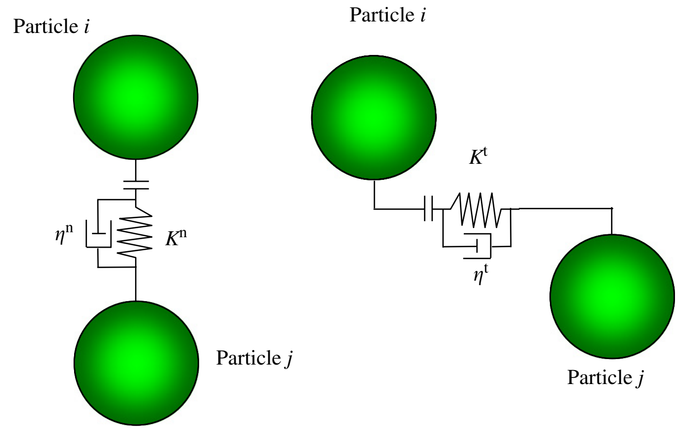

Fig. 1. Schematic drawing of Voigt elements between a pair of particles in normal and tangential directions.

$$\eta = 2\sqrt{mK} \tag{6}$$

The hydrodynamic contribution was taken into account through the shielding effect by existence of other particles. The hydrodynamic drag force acting on each constituent particle should be definitely smaller than that without other particles. It is plausible to consider the drag force acts only on the surface directly exposed to a flow not shielded by other particles. The practical way of effective surface correction is shown schematically in Fig. 2. The surface of objective particle was divided into small elements and the elements directly exposed to flows were discriminated. Then the drag force and torque imposed on elements were accumulated over exposed surface area S_i. The fluid velocity around a particle $\boldsymbol{u}$ and corresponding pressure P in an infinite fluid space are given be the following equation (Russel et al., 1989; Lamb, 1972):

$$\begin{aligned}\boldsymbol{u}(x) = {} & (\boldsymbol{E} + \Omega)\cdot x - \boldsymbol{E}\cdot\boldsymbol{r}\left(\frac{a}{r}\right)^5 - \frac{5}{2}\frac{\boldsymbol{rr}\cdot\boldsymbol{E}\cdot\boldsymbol{r}}{\boldsymbol{r}}\left(\frac{\boldsymbol{a}}{\boldsymbol{r}}\right)^3\left(1 - \frac{a^2}{r^2}\right) \\ & + \frac{a^3}{r^3}(\omega_i - \omega_0)\times\boldsymbol{r} + \frac{3\boldsymbol{a}}{4\boldsymbol{r}}\left(1 + \frac{a^2}{3r^2}\right)(\boldsymbol{v}_i - \boldsymbol{u}_0) \\ & + \frac{3\boldsymbol{a}}{4\boldsymbol{r}}\left(1 - \frac{a^2}{r^2}\right)\frac{\boldsymbol{r}\cdot(\boldsymbol{v}_i - \boldsymbol{u}_0)\boldsymbol{r}}{r^2}\end{aligned} \tag{7}$$

$$P(\boldsymbol{x}) = -\frac{5\mu a^3}{\boldsymbol{r}^3}\frac{\boldsymbol{r}\cdot\boldsymbol{E}\cdot\boldsymbol{r}}{\boldsymbol{r}^2} + \frac{3\mu a}{2r^2}(\boldsymbol{v}_i - \boldsymbol{u})\cdot\boldsymbol{r}_i \tag{8}$$

where $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{x}_i$ is the position vector of arbitrary point from the center of objective particle, $\boldsymbol{E}$ is the rate of strain tensor defined by $(\boldsymbol{\Gamma} + \boldsymbol{\Gamma}^{\mathrm{T}})/2$, $\boldsymbol{\Omega}$ is the vorticity tensor given by $(\boldsymbol{\Gamma} - \boldsymbol{\Gamma}^{\mathrm{T}})/2$, $\boldsymbol{\Gamma}$ is the velocity gradient tensor, $\boldsymbol{u}_0(=\boldsymbol{\Gamma}\cdot\boldsymbol{x})$ and ω_0 $(=\frac{1}{2}\nabla\times u_0)$ are velocity and vorticity vector without the particle, respectively.

In this work the height of deposit considering is on the order of 10 μm, thus it is plausible to consider that the deposits are within the boundary layer formed near the surface and undergo shear flows. Although the space was separated by the plate and thus fluid was