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Evaluation of lubrication force on colliding particles for DEM simulation of fluidized beds

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Abstract

"Lubrication force" arises from hydrodynamic pressure in the interstitial fluid being squeezed out from the space between two solid surfaces. In the previous DEM simulations of gas–solid flows this force has not been explicitly taken into account since it may introduce the famous "Stokes Paradox", which postulates that: Two solid surfaces can never make contact in a finite time in a viscous fluid due to the infinite "lubrication force" when the distance approaches zero at the last moment of contact. It is easy to imagine that lubrication effect is critical in liquid–solid systems, but it may not be negligible even in gas–solid systems of light and small particles. Although the lubrication theory has been well established in liquid–solid systems, its application in gas–solid systems should be used with caution because the assumptions adopted in the classical lubrication theory are only valid for high viscous systems. In the present study, these assumptions are examined and semi-theoretical expressions for lubrication force are proposed based on numerical analysis. The paradox of contactless collision due to infinite lubrication force is effectively avoided by considering surface roughness, non-continuum fluid effect and van der Waals force. The coefficient of restitution is defined as a criterion for evaluating the significance of lubrication effect in collisions of particles in fluidized beds. For demonstration the lubrication effect was evaluated for beds of FCC particles and GB (glass beads), with diameters ranging from 25 to 100 μm and initial approaching velocity from u_{mf} to u_t. The calculated restitution coefficient ranged from 0 to nearly 1 and clearly showed that lubrication force plays a significant role during a close encounter of two particles even in gas–solid systems.

Keywords: Lubrication force; DEM simulation; Collision; Stokes Paradox; Restitution coefficient

1. Introduction

The DEM (Discrete Element Method) treats the microscopic particle behavior by solving Newton's equations of motion for each particle. It has become a popular tool for granular material simulation and has been applied to a variety of problems. The soft sphere model, which was first proposed by Cundall and Struck [1], was introduced to gas–solid systems by Tsuji [2] in 1993. Subsequently, Horio et al. [3–8] successfully applied the method to solve industrial issues relevant to fluidized beds for particle agglomeration, combustion with immersed tube and polymerization. However, there still remains a serious empirism in how to include different interparticle forces in Newton's equation of motion plausibly and also in how to adjust values such as the coefficient of restitution and the spring constant. To develop DEM further for more realistic simulation, a more accurate and practical collision model should be constructed in which the lubrication effect is included.

Lubrication force is a hydrodynamic viscous force arising from radial pressure in the interstitial fluid being squeezed from the space between two close solid surfaces. It originally received considerable attention in tribology (e.g. Briscoe and McClune [9]; Safa and Gohar [10]). Recently, researchers in the field of filtration and coagulation have also examined the elastohydrodynamic collisions between spherical particles. Davis [11] obtained both analytical and numerical solutions for collisions between two smooth spheres surrounded by thin isoviscous liquid layers with

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consideration of dynamic deformation of particle surface. Subsequently, his research group developed the classical lubrication theory by taking into account the interparticle forces [12] and non-continuum fluid effect [13]. More recently, Thornton et al. [14] brought forward a simple analytical approximation based on a Hertzian-like profile for the elastic deformation of two spheres. Lian et al. [15] extended the lubrication theory to power–law fluid between rigid spheres and derived the analytical solutions for different flow index.

Although the lubrication theory was well established back in the 1900s, its application into DEM simulation of gas–solid flows has not been received sufficient attention. The well-known expression [11] for lubrication force $F_L=6\pi\mu R^2 v/h$ indicates its relationship with fluid viscosity μ, particle radius R, relative approaching velocity v and surface distance h. As the viscosity of air is much lower than that of liquid, the lubrication force is generally considered to be negligible compared with gravity, hydrodynamic drag force and interparticle forces. Moreover, the so-called "Stokes Paradox" that results in an infinite lubrication force when the surface distance approaches zero may also have been restricting its application to DEM simulations. Actually, however, even in gas–solid fluidization disregarding of lubrication effect is not acceptable for Geldart's A and B powders with relatively small Stokes numbers. In the realistic collisions, we have several practical and essential reasons to avoid the paradox of contactless collision such as consideration of surface roughness, treatment of fluid as a non-continuum in the molecular scale and consideration of the effect of van der Waals force within very close surface distance. Among them, the effect of surface roughness is the most practical one because the existence of surface roughness effectively prevents particle surfaces from approaching much closer. And even if the surfaces are assumed to be ideally smooth, a minimum molecular distance Z_0 of about 4×10^{-10}m due to the molecular repulsion will remain when the surfaces make "physical" contact [16]. When two surfaces approach to such small distances, the interstitial fluid cannot be treated as a continuum any longer according to Hocking's theory [17] and adhesive forces such as van der Waals force must be taken into account.

In the present work, the assumptions in the classical lubrication theory are re-examined since they were basically applicable for liquid–solid systems and semi-empirical expressions for lubrication force are proposed based on numerical calculations. According to the minimum approachable surface distance, three cases with and without considering non-continuum fluid effect and van der Waals force are investigated in order to construct a more accurate collision model. Calculated examples for restitution coefficient are presented for two typical bed materials often used in fluidized beds, FCC (Fluid Cracking Catalyst) particles and GB (glass beads) with diameters ranging from 25 to 100 μm and initial approaching velocity from u_{mf} to u_t, to evaluate the lubrication effect on the approaching process of two particles.

2. Theoretical development of lubrication theory

2.1. Examination of classical lubrication theory

As illustrated in Fig. 1, let us consider two identical elastic and spherical particles with radius R and mass m being immersed in a gaseous fluid and approaching each other. For the initial condition at $t=0$, we specify that the spheres start with a gap h_0 between their undeformed surfaces at $r=0$ and with a relative approaching velocity v_0. The minimum surface distance that can be approached is denoted as h_{min}. Only head-on collisions and no rotational movements are considered in this paper. And particles of the present interest are assumed to be rigid during approaching and separating stage according to Davis' theory [11].

The kinematic equations of movement are listed below:

$$\frac{dh}{dt} = -v(t) = -(v_1+v_2) \tag{1}$$

$$m\frac{dv}{dt} = -\sum F(t) = -F_L \tag{2}$$

where lubrication force F_L is considered to be the only dominant force in resultant force term when the surface distance is small compared with the particle radius.

The classical lubrication theory was originally established based on liquid–solid systems, in which the following assumptions were adopted:

(1) The initial gap size h_0, from which lubrication effect is considered to be significant, is assumed to be much smaller than particle radius (usually 0.01 R [11]);
(2) The upper limit of integration of pressure for lubrication force is extended from particle radius to infinity;
(3) Paraboloid approximation of undeformed surface is applied in order to get the simplified gap profile.

$$H(r,t) = h(0,t) + r^2/R \tag{3}$$

(4) The fluid is treated as a continuum no matter how close the two surfaces approach.

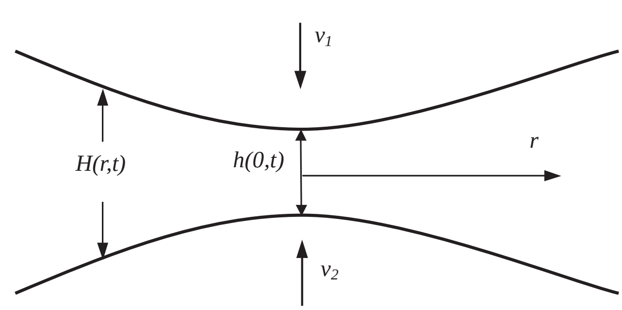

Fig. 1. Schematic of two approaching elastic and rigid spheres in a viscous fluid.

According to the classical lubrication theory (e.g. [11]), analytical expressions for interstitial pressure distribution and lubrication force can be derived as:

$$\frac{\partial p}{\partial r} = -\frac{6\mu r v}{H^3} \tag{4}$$

$$p(r,t) = \frac{3\mu R v}{2\left(h + r^2/R\right)^2} \tag{5}$$

$$F_{L,\infty} = \int_0^\infty 2\pi r p(r,t)\mathrm{d}r = \frac{3}{2}\pi\mu R^2 v/h. \tag{6}$$

The radial pressure distribution expressed by Eq. (5) indicates that the pressure decays rapidly to zero within a small radial distance in the so-called "inner region". The contribution of the pressure in the outer region to the integral of lubrication force can thus be reasonably neglected. Accordingly, the upper limit of integration can be effectively extended from R to infinity just to obtain the simplified analytical form of lubrication force. Also, within this small inner region, paraboloid approximation is sufficiently accurate.

However, these assumptions may not remain reasonable with regard to particle collisions in gas–solid systems. Among them, the initial gap size h_0 should be firstly checked to define the lubrication effect area. Order-of-magnitude estimates of different forces in case of FCC particles with radius of 25 μm and approaching velocity of terminal velocity u_t are indicated in Fig. 2. The drag force F_d was calculated under laminar conditions with a Reynolds number of about 0.293. An effective drag coefficient $C_D' = C_D \varepsilon^{-4.65}$ was adopted with a bed voidage ε of 0.9. It can be seen that from $h_0 = R$ the lubrication force should be taken into account compared with other forces such as gravity G and drag force F_d. The results agree well with Brenner's exact solutions [18] and hybrid approximation suggested by Leighton [19]. Thus, the particle radius can be regarded as a characteristic distance to judge whether the two particles have entered the so-called "lubrication effect area" or "near contact area", in which lubrication force should be included in the Newton's equation of motion. Out of this near contact area where particles are separated from each other widely, particle movements are dominated by hydrodynamic drag force and gravity, with lubrication force being neglected.

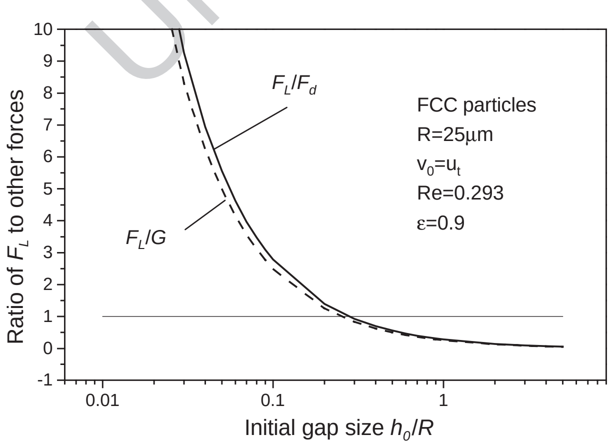

Fig. 2. Order-of-magnitude estimates of different forces.

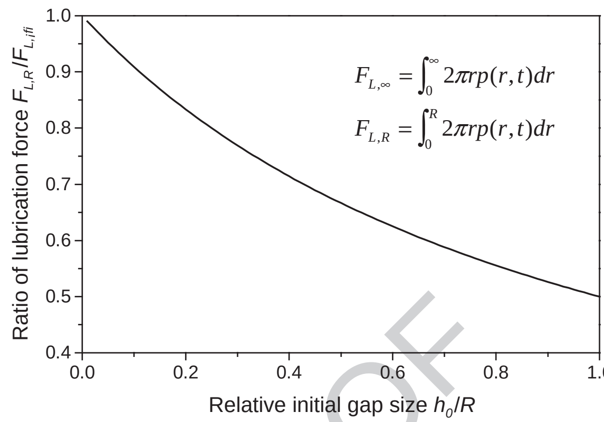

Fig. 3. Comparison of lubrication force applying different upper limit for integration (FCC particles, in air, R=25 μm, $v_0 = u_t$=0.098 m/s).

Fig. 3 shows the ratio of lubrication force integrated with different upper limit changing with the relative initial gap size. The actual lubrication force should be integrated over the particle surface:

$$F_{L,R} = \int_0^R 2\pi r p(r,t)\mathrm{d}r. \tag{7}$$

From Fig. 3, we can see that when h_0 is much smaller than the particle radius, the difference is not so significant. However, when h_0 increases to as large as the particle radius, the actual lubrication force from Eq. (7) is only half of that integrated from zero to infinity by Eq. (6). Therefore, the adoption of the upper limit as infinity is unreasonable when the lubrication effect area is as larger as the particle radius R.

For estimation of the error introduced by paraboloid approximation, numerical calculations for accurate pressure distribution and lubrication force were conducted under different initial gap size. Without the paraboloid approximation, the distance $H(r,t)$ between particle surfaces has the following accurate expression:

$$H(r,t) = h(0,t) + 2R - 2\sqrt{R^2 - r^2}. \tag{8}$$

By combining Eq. (8) with Eq. (4), one can obtain the pressure distribution numerically.

Fig. 4 shows that the numerical pressure distribution decays to zero much more slowly than the analytical solution. The contribution of pressure in the outer region to the lubrication force may play an important role

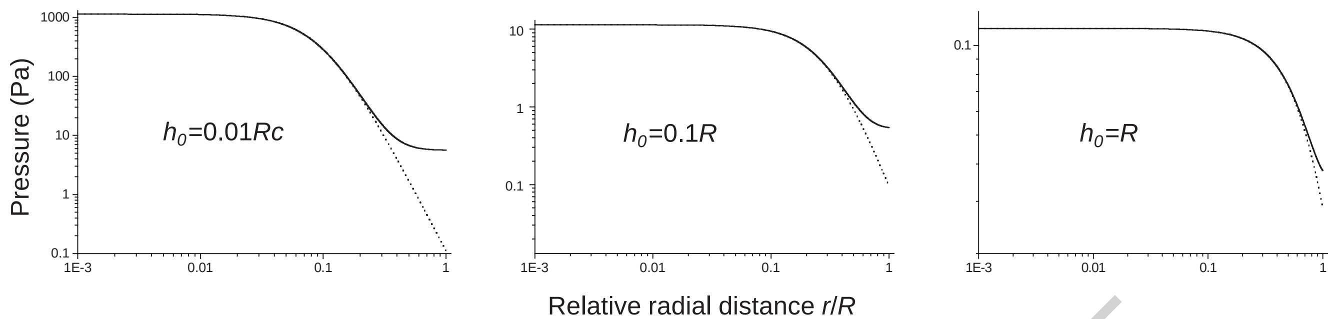

Fig. 4. Comparison of pressure distribution between numerical and analytical solutions (solid line: numerical solutions calculated from Eqs. (4) and (8); dotted line: analytical solutions calculated from Eq. (5)).

especially when h_0 is much smaller than particle radius. The relative magnitude of analytical and numerical solution for lubrication force along the radial direction is shown in Fig. 5. The analytical expression for lubrication force with various integration upper limits is based on paraboloid approximation.

$$F_{\mathrm{L,r,ana}} = \int_0^r 2\pi r p(r,t)\mathrm{d}r = \frac{3}{2}\pi\mu R^2 v\left(\frac{1}{h} - \frac{1}{h + r^2/R}\right). \tag{9}$$

Variation of $F_{\mathrm{L,r,ana}}$ with radial distance indicates the contribution of pressure within different radial distance to the lubrication force. We define the radial distance r^* as the radius of inner region and suppose that, within this inner region, the analytical solution has an accuracy of 90% of the accurate numerical solution. We found that the inner region expanded with the increase of gap size, thus making the analytical solution convincing in a wider region. When $h=R$, the analytical solution agrees well with the numerical one in the whole integration range from zero to R.

Finally, in gas–solid systems, the mean free path l_0 of gaseous molecules is in the order of 10^{-7} m, which is much larger than that of liquid molecules. Therefore, the assumption that the fluid remains a continuum may be broken when the surface distance is approached to such a magnitude that is comparable to the mean free path.

With the examination of the assumptions adopted in liquid–solid systems, we found that all of them were not valid when gas–solid systems are concerned. The exact surface distance, pressure profile and lubrication force should be solved numerically by combining Eqs. (4), (7) and (8).

2.2. Lubrication force and avoidance of "Stokes Paradox"

In the collision process between practical particles with roughness, the minimum approachable surface distance $h_{\min}$ is assumed to be determined by the height of surface roughness h_{r}. Accordingly, the maximum lubrication force corresponding to the moment at which physical contact occurs depends on the surface morphology of particles. When the surface roughness is of the same order of the mean free path of gaseous molecules, the interstitial fluid should be treated as a non-continuum. What's more, when its magnitude is comparable to the dominant range of adhesive forces, the effect of such forces on collision must be taken into account. According to the relative magnitude of minimum approachable surface distance $h_{\min}$, three cases are discussed below.

Case 1. $h_{\min} > l_0$

In this case, particles have large surface roughness that is much larger than the mean free path l_0 and the interstitial fluid can be reasonably regarded as a continuum.

Based on the numerical calculation results, the ratio of numerical solution to analytical one for lubrication force is found to be a function of the relative approaching distance

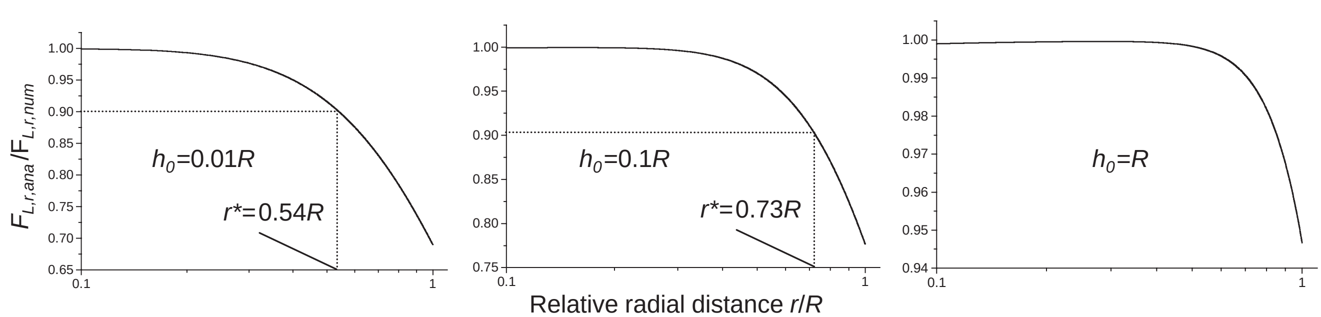

Fig. 5. Comparison of numerically and analytically calculated lubrication force with various integration upper limit. $F_{\mathrm{L,r,ana}} = \int_0^r 2\pi p_1(r,t)\mathrm{d}r$, where $p_1(r,t)$ has the analytical form of Eq.(5). $F_{\mathrm{L,r,num}} = \int_0^r 2\pi p_2(r,t)\mathrm{d}r$, where $p_2(r,t)$ is the numerically solved from Eqs.(4) and (8).

h/R. The relationship curve can be fitted by a two-order polynomial correlation with an error smaller than 1.5% in the range of $0.01<h/R<1$ (see Fig. 6).

$$K_1(h) = \frac{F_{\mathrm{L,num}}}{F_{\mathrm{L,ana}}} = 1.041 - 0.281\lg\frac{h}{R} - 0.035\lg^2\frac{h}{R} \tag{10}$$

where $F_{\mathrm{L,ana}}$ is the analytical expression for lubrication force integrated over the particle surface with paraboloid approximation.

$$F_{\mathrm{L,ana}}(h) = \int_0^R 2\pi r p \mathrm{d}r = \frac{3}{2}\pi\mu R^2 v\left(\frac{1}{h} - \frac{1}{h+R}\right). \tag{11}$$

Since the surface distance is unable to approach zero due to the prevention of surface roughness, the continuous increase of lubrication force in the approaching process is stopped when the tip of roughness makes contact. Hence, the infinite lubrication force cannot be reached and the "Stokes Paradox" is accordingly avoided.

Case 2. $Z_0<h_{\min}<l_0$

Particles in this case have smaller surface roughness compared with the mean free path. So the non-continuum fluid effect should be considered in the last stage of approaching.

Maxwell slip theory, which was initially introduced by Hocking [17] in 1973, is adopted in the present paper to treat the interstitial fluid as a non-continuum. Different from Eq. (4) for continuum fluid case, the pressure profile in the non-continuum fluid can be expressed by [17]:

$$\frac{\partial p}{\partial r} = -\frac{6\mu r v}{H^2(H+6l_0)} \tag{12}$$

where l_0 is the mean free path of gaseous molecules.

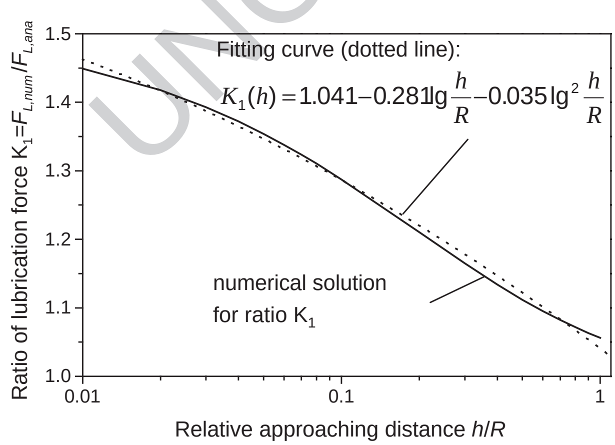

Fig. 6. Fitting curve of the ratio of numerical lubrication force to an analytical one (FCC particles, in air, $R=25$ μm, $v_0=u_t$, $h_0=R$, $F_{\mathrm{L,ana}}$ is calculated from Eq. (11) with paraboloid approximation). Numerical solution for ratio K1 Fitting curve (dotted line).

Similarly with Case 1, another semi-empirical correlation is proposed here with a relative error smaller than 1% in the range of $h/R<0.01$.

$$K_2(h) = \frac{F_{\mathrm{L,num,slip}}}{F_{\mathrm{L,ana,slip}}} = 1.309 - 0.082\lg\frac{h}{R} - 0.009\lg^2\frac{h}{R} \tag{13}$$

$$F_{\mathrm{L,ana,slip}} = \frac{\pi\mu R^2 v}{12 l_0^2}\left[(h+6l_0)\ln\left(\frac{h+6l_0}{h}\right) - (h+R+6l_0) \times\ln\left(\frac{h+R+6l_0}{h+R}\right)\right]. \tag{14}$$

From Eq. (14) we can find that when $l_0<<h$, the expression of $F_{\mathrm{L,ana,slip}}$ converges to $F_{\mathrm{L,ana}}$ in Eq. (11), and when $l_0>>h$, the expression of $F_{\mathrm{L,ana,slip}}$ converges to:

$$F_{\mathrm{L,ana,slip}} = \frac{\pi\mu R^2 v}{2l_0}\ln\left(\frac{6l_0}{h}\right), \quad l_0 \gg h. \tag{15}$$

The above expression shows that the increase of the lubrication force is slowed down because its magnitude is only proportional to the logarithm of the inverse of the gap size. Therefore, treatment of the fluid as a non-continuum also helps us avoid the paradox of the infinite lubrication force.

Case 3. $h_{\min}$ is comparable to Z_0

When the surface roughness is so small that the minimum approachable distance is of the same order of the repulsive molecular distance $Z_0=4*10^{-10}$ m, which is the dominant range of adhesive forces, these forces such as van der Waals force F_{vw} should be taken into account. In this case, the van der Waals force ought to be included in the resultant force term in the kinematic Eq. (2).

$$m\frac{\mathrm{d}v}{\mathrm{d}t} = -\sum F(t) = -(F_{\mathrm{L}} - F_{\mathrm{vw}}) \tag{16}$$

where lubrication force F_{L} can be calculated by applying Eq. (13) with the approximation of K_2 to be 1.5, and van der Waals force F_{vw} is expressed by

$$F_{\mathrm{vw}} = -\frac{AR}{12h^2} \tag{17}$$

where A is the Hamaker constant of the particle material.

As van der Waals force is inversely proportional to the square of the distance, its magnitude increases dramatically when the distance approaches Z_0. The variation of lubrication force, van der Waals force and the resultant net force along with surface distance are shown in Fig. 7. Under the condition that the net force $F_{\mathrm{net}}=F_{\mathrm{L}}-F_{\mathrm{vw}}=0$, we define a critical "collapse distance" h_{collapse}, above which the particles resist approaching to each other due to the lubrication force but below which, on the contrary, the

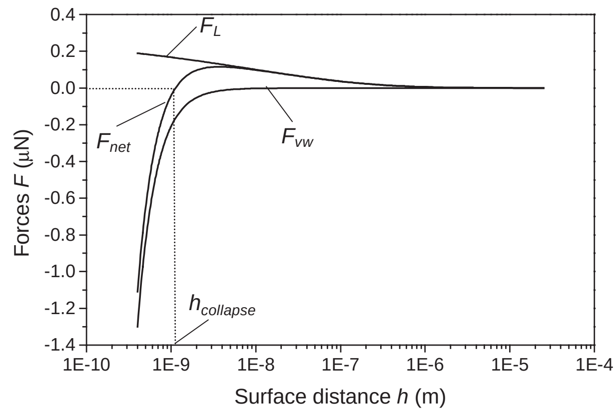

Fig. 7. Variation of lubrication force, van der Waals force and resultant net force with approaching surface distance (GB particles, $d_p=50$ μm, $v_0=u_t/5$, $h_0=R$).

particles collapse and make contact in the aid of van der Waals force. Therefore, the consideration of van der Waals force in the very last approaching stage essentially saves us from the paradox of contactless collision.

The collapse distance can be solved from the following equation:

$$\frac{3}{4}\frac{\pi\mu R^2 v}{l_0}\ln\frac{6l_0}{h_{\text{collapse}}} = \frac{AR}{12h_{\text{collapse}}^2}. \tag{18}$$

In the case of GB with diameter of 50 μm and approaching velocity of $u_t/5$, this collapse distance can be estimated to be $h_{\text{collapse}}=10^{-9}$ m.

By deriving the relationship of relative velocity with surface distance and substituting it into Eq. (18), we can get the dimensionless correlation:

$$\hat{E}St^2 = \frac{1}{4}\frac{l_0}{Z_0}\hat{h}_{\text{collapse}}^2\ln\frac{6}{\hat{h}_{\text{collapse}}}\left(St + \frac{1}{4}\hat{h}_0\ln\frac{\hat{h}_0}{16.3}\right) \tag{19}$$

where the dimensionless parameters are defined as:

$$\hat{h} = \frac{h}{l_0}, \quad St = \frac{mv_0}{6\pi\mu R^2}, \quad \hat{E} = \frac{E}{\frac{1}{2}mv_0^2} = \frac{AR}{6Z_0 m v_0^2} \tag{20}$$

where E is the depth of the attractive potential well due to van der Waals force:

$$E = -\int_{Z_0}^{\infty}\frac{AR}{12h^2}\mathrm{d}h = \frac{AR}{12Z_0}. \tag{21}$$

$\hat{h}$ is the relative distance compared with the mean free path, Stokes number, St, provides a measure of the inertia of an isolated particle relative to the viscous force and $\hat{E}$ is the dimensionless adhesion energy compared with initial kinetic energy.

Fig. 8 shows contours of the collapse distance with dimensionless parameters. The Y-coordinate $\hat{E}St^2 = \frac{A}{216\pi^2 Z_0 \mu^2 R^3}$ represents only the physical properties of fluid and particles, being independent of approaching velocity. With respect to a certain condition of particle and fluid, the collapse distance decreases with increase of Stokes number, indicating that the lubrication force dominates the particles' movement when the Stokes number of particles is large. Under the constant Stokes number, the collapse distance increases with increase of dimensionless adhesive energy $\hat{E}$. This means that with increasing Hamaker constant, the dominant range of van der Waals force which is smaller than h_{collapse} expands wider.

2.3. Effective restitution coefficient

The lubrication effect is actually a kind of damping effect, causing kinetic energy dissipation during both approaching and separating stage. Restitution coefficient, which represents the energy loss during collision process, is usually defined as the ratio of the normal relative velocity at the instant of rebound to that at the instant of contact. However, if we consider that the collision process begins when the particles enter the lubrication effect area and ends when the surface distance recovers to the initial gap size, the definition of restitution coefficient can be extended as the ratio of normal velocity at the instant of escaping from this area (v_e) to that at the instant of entering this area (v_0). Thus restitution coefficient can be regarded as a criterion for evaluating the lubrication effect during approaching and separating process.

Combining Eqs.), (1), (2), (10)-(14) to eliminate the time term and integrating in the approaching and separating stage, we can obtain the expression for the restitution coefficient e.

$$e = e_c - \frac{1+e_c}{2St}St_e^* \tag{22}$$

where e_c is the restitution coefficient due to particle deformation in the collision process. If we assume that the

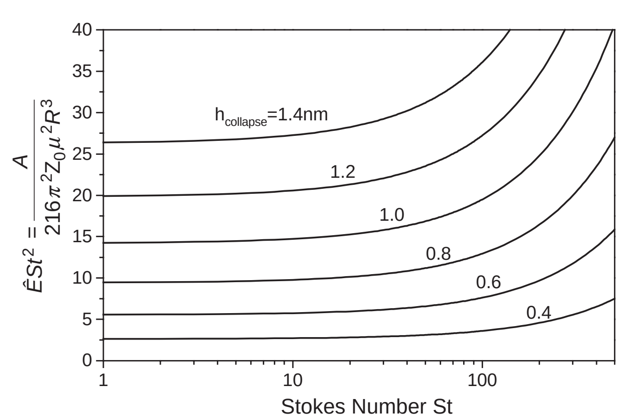

Fig. 8. Contour of collapse distance with dimensionless parameters (GB, in air, $R=25$ μm, range of St: 1~500).

collision process is an elastic one with e_c being equal to unity, Eq. (22) can be simplified into:

$$e = 1 - \frac{St_e^*}{St} = 1 - \frac{2St_c^*}{St} \tag{23}$$

where the two critical Stokes number are defined as:

$$St_c^* = \frac{mv_c^*}{6\pi\mu R^2}, \quad St_e^* = \frac{mv_e^*}{6\pi\mu R^2} \tag{24}$$

where v_c^* is called "critical contact velocity". Particles with initial approaching velocity v_0 smaller than v_c^* cannot make contact due to the repulsive lubrication force; v_e^* is called "critical escape velocity". Particles with $v_0 > v_c^*$ but $v_0 < v_e^*$, however have sufficient kinetic energy to make contact, yet cannot escape from the lubrication effect area due to the attractive lubrication force during the separating stage and will be brought to rest.

By derivation, St_e^* has the following expression:

$$St_e^* = f(h_0) - f(h_{\min}) = 2St_c^* \tag{25}$$

where $f(h)$ is called "characteristic function", h_0 is considered to be equal to particle radius and $h_{\min}$ is practically determined by surface roughness.

For Case 1 with continuum fluid:

$$f_1(h) = 0.962\ln\left(\frac{h}{h+R}\right) - 0.079\ln^2\left(\frac{h}{h+R}\right) - 0.004\ln^3\left(\frac{h}{h+R}\right). \tag{26}$$

For Case 2 with non-continuum fluid:

$$f_2(h) = \frac{1}{36}\left(6+\frac{h}{l_0}\right)^2\ln\left(1+\frac{6l_0}{h}\right) - \frac{1}{36}\left(6+\frac{h+R}{l_0}\right)^2\ln\left(1+\frac{6l_0}{h+R}\right) - \ln\left(1+\frac{R}{h}\right) - \frac{R}{6l_0}. \tag{27}$$

For Case 3 with non-continuum fluid and van der Waals force:

$$St_e^* = f_3(h_0) - f_3\left(h_{\text{collapse}}\right), \quad f_3(h) = f_2(h). \tag{28}$$

In Case 3, the characteristic function $f_3(h)$ is the same as that for Case 2 (Eq. (27)). However, the minimum approachable distance $h_{\min}$ in Eq. (25) should be replaced by the collapse distance h_{collapse} because particles with enough inertia to approach h_{collapse} can further make contact in the aid of van der Waals force even if the velocity at this moment has decreased to zero. Nevertheless, the effect of van der Waals force on the restitution coefficient is not so significant since most of the energy loss is dissipated by lubrication force before they nearly make contact. This can also be demonstrated by the similar value of $f_2(h_{\min})$ and $f_3(h_{\text{collapse}})$ in Eqs. (25) and (28).

3. Calculated examples and discussion

In the present paper, two typical powders for fluidized bed processes, i.e., FCC particles and GB (Glass Bead), are adopted to evaluate the lubrication effect on collision process. The particle size ranges from 25 to 100 μm corresponding to Geldart's A and B classification and the initial approaching velocity varies from u_{mf} to u_{t}. The physical properties of particles and fluid are listed in Table 1.

3.1. Case 1: FCC particles with large surface roughness

From observation of the surface morphology of FCC particles by laser microscopy, the surface roughness of each tested particle is approximately one tenth of the particle radius. Within the range of particle size investigated in this paper, $h_{\min}$ is much larger than the mean free path of air molecules. Therefore, the interstitial fluid can be reasonably treated as a continuum in the case of FCC particles.

Fig. 9 shows the variation of lubrication force and relative velocity during the approaching and separating stage with the surface distance. At the moment when the surface distance equals to the surface roughness, physical contact between the surfaces occurs. Subsequently, the separating stage begins until the surface distance returns to the initial value h_0. Due to the energy dissipation by the lubrication force both in approaching and separating stage, the relative velocity keeps decreasing in the whole process. Lubrication force increases more rapidly when the surfaces approach closer. At the moment of contact in this example, its magnitude increases to a maximum value which is about 20 times of its initial value at $h = h_0$.

Fig. 10 shows how restitution coefficient varies with initial approaching velocity ranging from u_{mf} to u_{t}. Results applying classical lubrication theory are also displayed using

Table 1
Physical properties of particles and fluid

	FCC	GB
Particles		
Particle diameter d (μm)	25∼100	25∼100
Particle density ρ_p (kg/m^3)	1400	2650
Young's Modulus E (N/m^2)	1.0×10^{11}	8.0×10^{10}
Poisson's ratio ν	0.28	0.3
Roughness h_r (m)*	1/10 of the particle radius	1/1000 of the particle radius
Hamaker constant A (J)	–	1.0×10^{-19}
Fluid: Air at p = 1 atm, T = 300 K		
Viscosity μ (Pa s)	1.94×10^{-5}	
Density ρ_f (kg/m^3)	1.16	
Mean free path l_0 (m)	7.15×10^{-8}	

* Surface roughness of particles is estimated based on the optical observation of surface morphology using laser microscopy and SEM.

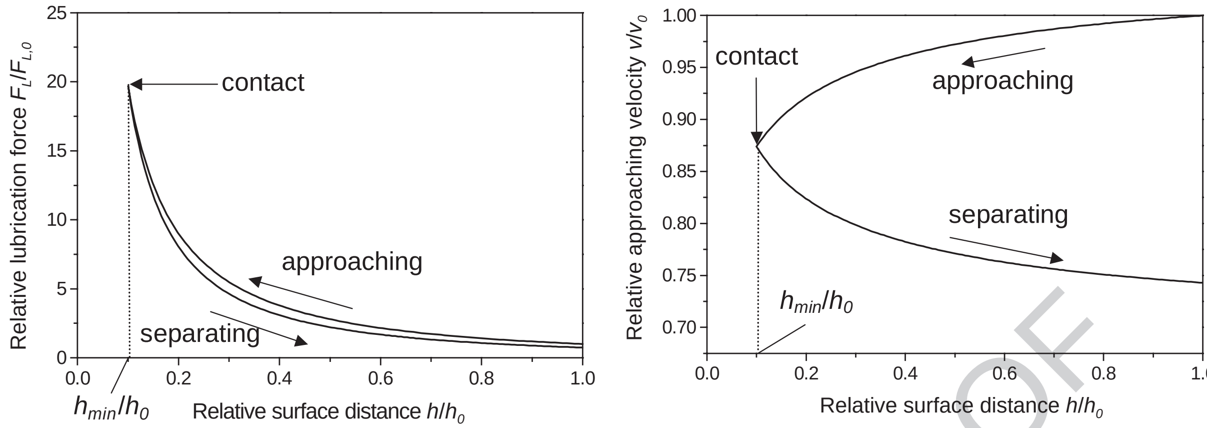

Fig. 9. Variation of lubrication force and approaching velocity with relative surface distance (FCC particles, $d_p=50$ μm, $v_0=u_t/5$, $h_0=R$, $h_{min}=h_r=0.1\ R$).

dotted lines for comparison. With the increase of initial velocity, restitution coefficient approaches to unity, indicating that lubrication effect is not so significant at high velocities. Nevertheless, when the initial velocity is smaller than the critical escape velocity v_e^*, e decreases to zero. Particles with initial velocity of u_{mf} and $u_t/50$ which are smaller than v_c^* do not have enough inertia to make contact and will come to rest in the approaching stage. Yet particles with an initial velocity of $u_t/20$ can make contact but do not have enough inertia to escape from the "lubrication effect area" and will come to rest in the separating stage. Therefore, collisions with an initial approaching velocity less than v_e^* will result in agglomeration. The results calculated by classical lubrication theory show a similar tendency and smaller values of a restitution coefficient due to the assumption of the upper limit of infinity in the integration of the lubrication force.

Results of restitution coefficient with different particle size and different initial approaching velocity are shown in Fig. 11. It can be found that under the same initial velocity, the effect of the lubrication force on larger particles is less significant than on smaller particles. The independent effects of particle size and initial approaching velocity on the collision process can be included in the consideration of Stokes numbers. As can be seen from Fig. 12, the effect of lubrication force on particles with larger St is less significant. The lubrication effect can be completely neglected when the Stokes number is larger than 1000. Fig. 12 also shows the influence of different surface roughness on the restitution coefficient. For the same Stokes number, the lubrication effect on the collision is more significant in case of smoother particles.

3.2. Case 2: GB with small surface roughness

Glass beads with surface roughness that is approximately equal to 1/1000th of the particle radius are much smoother than FCC particles. The particle surfaces can approach to a much closer distance so that the lubrication effect is more significant and the fluid should be treated as a non-continuum in the last approaching stage.

Fig. 13 shows the comparison of lubrication force along with surface distance with and without considering the non-continuum fluid effect. It can be seen that the magnitude of lubrication force decreases greatly when the surface distance is of the same order of a mean free path of air by taking into

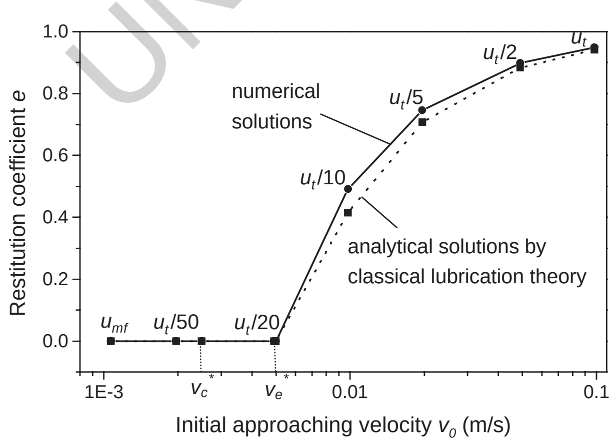

Fig. 10. Variation of restitution coefficient with initial approaching velocity (FCC particles, $d_p=50$ μm, $h_0=R$, $h_{min}=h_r=0.1\ R$).

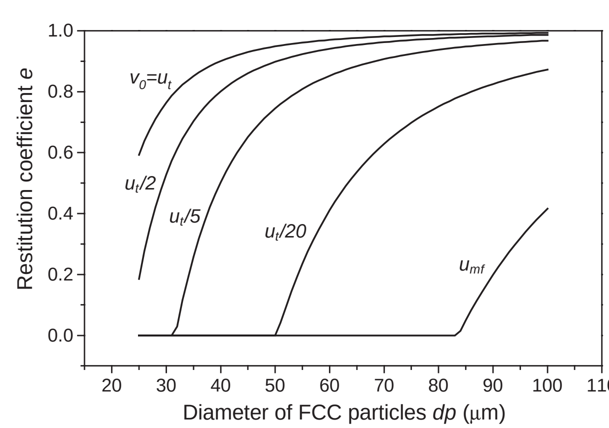

Fig. 11. Restitution coefficient with different size of FCC particles and different initial approaching velocity (FCC particles, $h_0=R$, $h_{min}=h_r=0.1\ R$, velocity range: $u_{mf}\sim u_t$; diameter range: 25~100 μm).

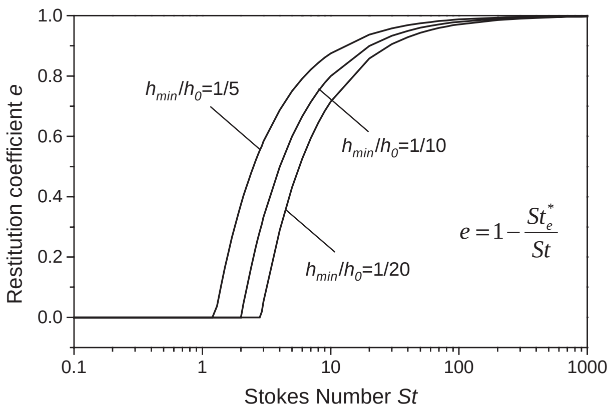

Fig. 12. Variation of restitution coefficient with Stokes numbers and different surface roughness (FCC particles, $h_0=R$, $h_{\min}=h_r$).

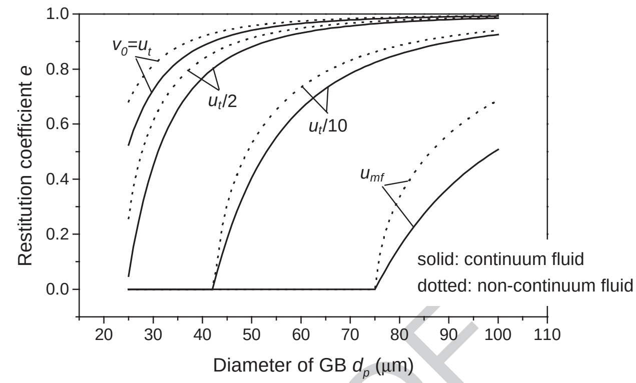

Fig. 14. Comparison of restitution coefficient calculated by continuum and non-continuum fluid model (GB particles, $h_0=R$, $h_{\min}=h_r=0.001$ R velocity range: $u_{mf} \sim u_t$; diameter range: 25∼100 μm).

account the non-continuum fluid effect. Therefore, treatment of the fluid as a non-continuum in the last approaching stage significantly slows down the increase of lubrication force to infinity.

A comparison of the restitution coefficient of different sized GB under different initial approaching velocities is shown in Fig. 14. Results indicate that lubrication effect on GB collisions cannot either be neglected especially for smaller particles and lower initial approaching velocity. The differences of restitution coefficient with and without non-continuum effect also indicate that consideration of non-continuum effect weakens the lubrication effect and thus lead to an increase in the restitution coefficient.

3.3. Case 3: smooth GB without surface roughness

In most DEM simulations, GB is assumed to be ideally smooth without surface roughness. However, even in this case, the paradox of contactless collision can be essentially avoided by the attractive interaction of adhesive forces in the range of distance smaller than h_{collapse}. This collapse distance h_{collapse} can thus be regarded as the minimum approachable surface distance $h_{\min}$.

Fig. 15 shows the calculated results of the restitution coefficient with and without considering the effects of non-continuum fluid and van der Waals force. Comparing with Fig. 14, we can find that the differences between two sets of results are much larger because, with the assumption of smooth GB surface, particles can approach more closely so that the effect of non-continuum fluid may be more significant.

4. Conclusions

Although the classical lubrication theory has been well established in liquid–solid systems, its application into gas–solid systems has not received enough attention. The assumptions adopted in the previous lubrication theory do not remain reasonable as to gas–solid systems based on the numerical analysis. The lubrication effect area in gas–solid systems can be as large as the particle radius. The numerical calculation results show that the pressure distribution in the outer region cannot be neglected and their contribution to lubrication force is related to the relative surface distance. Semi-empirical expressions for lubrication force with and

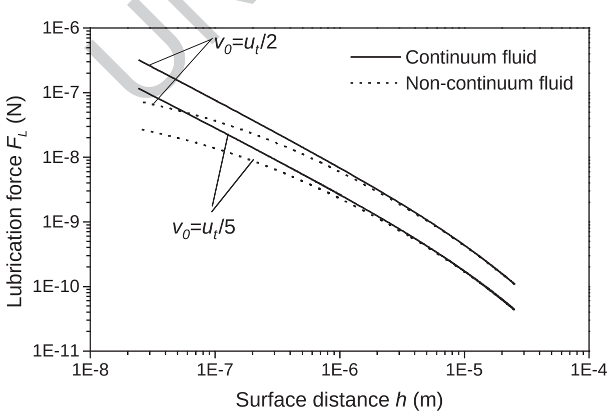

Fig. 13. Variation of lubrication force with surface distance applying continuum fluid model and non-continuum fluid model (GB particles, $d_p=50$ μm, $h_0=R$, $h_{\min}=h_r=0.001$ R).

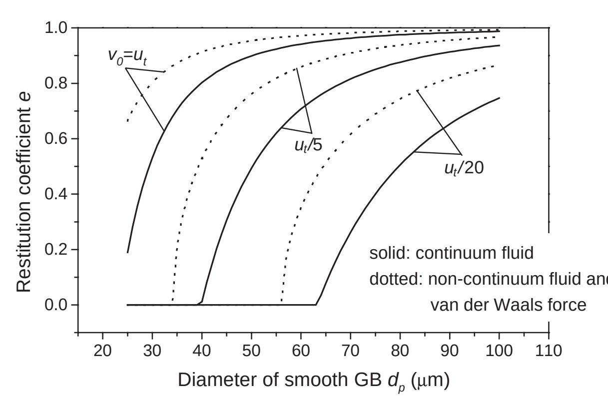

Fig. 15. Restitution coefficient with and without non-continuum fluid effect and van der Waals force (GB particles, $h_0=R$, $h_{\min}=h_{\text{collapse}}$, velocity range: $u_{mf} \sim u_t$; diameter range: 25∼100 μm).

without considering non-continuum fluid effect are proposed according to the numerical analysis.

Surface roughness of practical particles helps us avoid the classical “Stokes Paradox” since it prevents particles from approaching to a closer distance. Moreover, in the last approaching stage where the surface distance is of the order of the mean free path of fluid, the interstitial fluid should be treated as a non-continuum, thus slowing down the increase of lubrication force. Finally, within a critical collapse distance where van der Waals force dominates over lubrication force, the paradox of contactless collision is essentially avoided since the particles can be driven together to make contact in the aid of van der Waals force.

Restitution coefficient is adopted as a criterion for evaluating the lubrication effect on collision process. It is a strong function of Stokes number of isolated particle and critical Stokes number that can be determined by corresponding characteristic functions. The lubrication effect is more pronounced for particles with smaller Stokes numbers. Calculation results clearly show that the lubrication effect cannot be neglected during the collision process in gas–solid systems with FCC and GB of particle sizes ranging from 25 to 100 μm and initial approaching velocity from u_{mf} to u_{t}.

Further research should be aiming at incorporating lubrication force and an effective restitution coefficient defined in this paper into DEM simulations with a more accurate collision model.

Nomenclature

A	Hamaker constant, J
d_{p}	Particle diameter, μm
E	Attractive potential, J
e	Restitution coefficient in Eq. (22)
e_{c}	Restitution coefficient by deformation
F_{d}	Drag force, N
F_{L}	Lubrication force, N
F_{vw}	Van der Waals force, N
F_{net}	Resultant net force, N
G	Gravity, N
H	Surface distance, m
h	Surface distance at $r=0$, m
h_0	Initial surface distance at $r=0$, m
h_{min}	Minimum surface distance, m
h_{r}	Surface roughness, m
h_{collapse}	Critical collapse distance, m
K_1	Correction factor in Eq. (10)
K_2	Correction factor in Eq. (13)
l_0	Mean free path of molecules, m
m	Particle mass, kg
P	Hydrodynamic pressure, Pa
R	Particle radius, m
r	Radial distance in Fig. 1, m
r^*	Radius of inner region, m
St	Stokes number
St_{c}^*	Critical contact Stokes number
St_{e}^*	Critical escape Stokes number
u_{mf}	Minimum fluidized velocity, m/s
u_{t}	Terminal velocity, m/s
v	Relative approaching velocity, m/s
v_0	Initial approaching velocity, m/s
v_{c}^*	Critical contact velocity, m/s
v_{e}^*	Critical escape velocity, m/s
Z_0	Repulsive molecular distance, m

Greek letters

ε	Bed voidage
μ	Viscosity of fluid, Pa s
ρ_{p}	Particle density, kg/m^3
ρ_{f}	Fluid density, kg/m^3

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