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Granular Shear Flows of Flexible Rod-like Particles

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Abstract. Flexible particles are widely encountered in nature, e.g., stalks of plants, fiberglass particles, and ceramic nanofibers. Early studies indicated that the deformability of particles has a significant impact on the properties of granular materials and fiber suspensions. In this study, shear flows of flexible particles are simulated using the Discrete Element Method (DEM) to explore the effect of particle flexibility on the flow behavior and constitutive laws. A flexible particle is formed by connecting a number of constituent spheres in a straight line using elastic bonds. The forces/moments due to the normal, tangential, bending, and torsional deformation of a bond resist the relative movement between two bonded constituent spheres. The bond stiffness determines how difficult it is to make a particle deform, and the bond damping accounts for the energy dissipation in the particle vibration process. The simulation results show that elastically bonded particles have smaller coefficients of restitution compared to rigidly connected particles, due to the fact that kinetic energy is partially converted to potential energy in a contact between flexible particles. The coefficient of restitution decreases as the bond stiffness decreases and the bond damping coefficient increases. As a result, smaller stresses are obtained for granular flows of the flexible particles with smaller bond stiffness and larger bond damping coefficient.

Keywords: Flexible Rod-like Particle; Granular Shear Flow; Discrete Element Method
PACS: 47.57.Gc

INTRODUCTION

Flexible rod-like particles and filamentous fibers have been utilized to manufacture fabrics, fiber-reinforced composites, biomass fuels, tobaccos, and papers. The improvement of the manufacturing procedure and the product quality depends on better understanding of the dynamics and rheology of fibers and fiber suspensions in these industrial processes [1]. In this work, a computational model of damped flexible particles based on the Discrete Element Method (DEM) is presented and employed to simulate granular shear flows of flexible rod-like particles. The effects of bond stiffness and bond damping on the coefficients of restitution for collisions and the particle phase stresses for shear flows are studied.

COMPUTATIONAL MODEL

An elongated rod-like particle is formed by connecting a number of identical spheres in a straight line using elastic bonds. Two ends of a single bond, which are fixed on the centers of two neighboring spheres, translate and rotate with the spheres. Thus, the relative movement of constituent spheres in a composite particle leads to the deformation of the bonds and also the particle. In return, the bond forces/moments are generated and exerted on the spheres to resist the deformation. According to the bonded-particle model [2], the bond forces/moments can be calculated incrementally as follows:

$$dF_n^b = K_{\mathrm{n}}^{\mathrm{b}} d\delta_n^r = \frac{EA}{l_b} v_n^r dt \ , \tag{1}$$

$$dF_t^b = K_{\mathrm{t}}^{\mathrm{b}} d\delta_t^r = \frac{GA}{l_b} v_t^r dt \ , \tag{2}$$

$$dM_n^b = K_{\mathrm{tor}}^{\mathrm{b}} d\theta_n^r = \frac{GI_p}{l_b} \omega_n^r dt \ , \tag{3}$$

$$dM_t^b = K_{\mathrm{ben}}^{\mathrm{b}} d\theta_t^r = \frac{EI}{l_b} \omega_t^r dt \ , \tag{4}$$

in which, dF_n^b, dF_t^b, dM_n^b, and dM_t^b are the incremental normal force, tangential force, torsional moment, and bending moment, respectively, and $d\delta_n^r$, $d\delta_t^r$, $d\theta_n^r$, and $d\theta_t^r$ are the incremental normal deformation, tangential deformation, normal angular deformation, and tangential angular deformation, respectively, of the bond. Thus, $K_{\mathrm{n}}^{\mathrm{b}}$, $K_{\mathrm{t}}^{\mathrm{b}}$, $K_{\mathrm{tor}}^{\mathrm{b}}$, and $K_{\mathrm{ben}}^{\mathrm{b}}$ represent the normal, shear, torsional, and bending stiffnesses, respectively, of the bond. The cylindrical bond of Young's modulus E and shear modulus G has a radius r_{b}, a length $l_{\mathrm{b}} = 2r_{\mathrm{s}}$, a cross sectional area $A = \pi r_{\mathrm{b}}^2$, an area moment of inertia $I = \pi r_{\mathrm{b}}^4/4$, and a polar area moment of inertia $I_{\mathrm{p}} = \pi r_{\mathrm{b}}^4/2$. In the present model, the bond radius r_{b} is the same as the radius of the constituent sphere r_{s}, and the bond Young's modulus E and shear modulus G

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are correlated through the Poisson's ratio ξ as $E = 2(1+\xi)G$. The incremental relative displacements can be calculated based on the corresponding relative velocities ($v_{\mathrm{n}}^{\mathrm{r}}$, $v_{\mathrm{t}}^{\mathrm{r}}$, $\omega_{\mathrm{n}}^{\mathrm{r}}$ and $\omega_{\mathrm{t}}^{\mathrm{r}}$) and the time step dt.

The movement of individual constituent spheres in each rod-like particle is governed by Newton's second law of motion, i.e.,

$$m_{\mathrm{s}} \frac{\mathrm{d}^2 \boldsymbol{x}_{\mathrm{s}}}{\mathrm{d}t^2} = \boldsymbol{F}^{\mathrm{c}} + \boldsymbol{F}^{\mathrm{b}} + m_{\mathrm{s}}\boldsymbol{g} + \boldsymbol{F}_{\mathrm{d}}^{\mathrm{c}} + \boldsymbol{F}_{\mathrm{d}}^{\mathrm{b}}, \tag{5}$$

$$J_{\mathrm{s}} \frac{\mathrm{d}^2 \boldsymbol{\theta}_{\mathrm{s}}}{\mathrm{d}t^2} = \boldsymbol{M}^{\mathrm{c}} + \boldsymbol{M}^{\mathrm{b}} + \boldsymbol{M}_{\mathrm{d}}^{\mathrm{c}} + \boldsymbol{M}_{\mathrm{d}}^{\mathrm{b}}, \tag{6}$$

in which, $\boldsymbol{x}_{\mathrm{s}}$ and $\boldsymbol{\theta}_{\mathrm{s}}$ are the translational displacement and angular displacement, respectively, of the sphere of mass m_{s} and moment of inertia J_s. The translational motion of the sphere is driven by the contact force $\boldsymbol{F}^{\mathrm{c}}$ exerted by the spheres from the other composite particles, the bond force $\boldsymbol{F}^{\mathrm{b}}$ exerted by the bonds connecting to it, and the gravitational force $m_{\mathrm{s}}\boldsymbol{g}$. The contact force between the spheres from two different composite particles, $\boldsymbol{F}^{\mathrm{c}}$, can be described by Hertz-Mindlin-Deresiewicz theory [3] and the bond force $\boldsymbol{F}^{\mathrm{b}}$ can be calculated incrementally based on Eqs.(1)-(2). The moment $\boldsymbol{M}^{\mathrm{c}}$ arises from the tangential component of contact forces $\boldsymbol{F}^{\mathrm{c}}$, and $\boldsymbol{M}^{\mathrm{b}}$ represents the bond moment induced by the shearing, bending, and twisting deformation of the bond.

In Eq.(5), the contact damping force $\boldsymbol{F}_{\mathrm{d}}^{\mathrm{c}}$ is introduced to account for the energy dissipation when two composite particles collide. The normal and tangential contact damping forces can be written as

$$F_{\mathrm{dn}}^{\mathrm{c}} = \beta_{\mathrm{c}} \sqrt{2 m_{\mathrm{p}} K_{\mathrm{n}}^{\mathrm{c}}}\, v_{\mathrm{n}}^{\mathrm{c}}\,, \tag{7}$$

$$F_{\mathrm{dt}}^{\mathrm{c}} = \beta_{\mathrm{c}} \sqrt{2 m_{\mathrm{p}} K_{\mathrm{t}}^{\mathrm{c}}}\, v_{\mathrm{t}}^{\mathrm{c}}\,, \tag{8}$$

in which, m_{p} is the mass of a composite particle. The contact normal stiffness $K_{\mathrm{n}}^{\mathrm{c}}$ and tangential stiffness $K_{\mathrm{t}}^{\mathrm{c}}$ are based on the sphere-sphere contact and given in [3]. The variables $v_{\mathrm{n}}^{\mathrm{c}}$ and $v_{\mathrm{t}}^{\mathrm{c}}$ represent the normal and tangential components, respectively, of the relative velocity at the contact point. The contact damping coefficient β_{c}, which leads to a coefficient of restitution of 0.95 for two rigid particle contact, is fixed for all the simulations with flexible particles in this study. In Eq.(6), $\boldsymbol{M}_{\mathrm{d}}^{\mathrm{c}}$ is the moment arising from the contact damping force $\boldsymbol{F}_{\mathrm{d}}^{\mathrm{c}}$.

Analogous to contact damping, the bond damping can be proposed to take into account energy dissipation as the elastic wave propagates through the bonds. Thus, the bond damping forces/moments are assumed to follow,

$$F_{\mathrm{dn}}^{\mathrm{b}} = \beta_{\mathrm{b}} \sqrt{2 m_s K_{\mathrm{n}}^{\mathrm{b}}}\, v_n^r\,, \tag{9}$$

$$F_{\mathrm{dt}}^{\mathrm{b}} = \beta_{\mathrm{b}} \sqrt{2 m_s K_{\mathrm{t}}^{\mathrm{b}}}\, v_t^r\,, \tag{10}$$

$$M_{\mathrm{dn}}^{\mathrm{b}} = \beta_{\mathrm{b}} \sqrt{2 J_s\, K_{\mathrm{tor}}^{\mathrm{b}}}\, \omega_n^r\,, \tag{11}$$

$$M_{\mathrm{dt}}^{\mathrm{b}} = \beta_{\mathrm{b}} \sqrt{2 J_s K_{\mathrm{ben}}^{\mathrm{b}}}\, \omega_t^r\,, \tag{12}$$

in which, m_s and J_s are the mass and moment of inertia, respectively, of the constituent sphere. The bond damping coefficient β_{b} varies in the range 0-1 to determine the energy dissipation rate. The bond damping force $\boldsymbol{F}_{\mathrm{d}}^{\mathrm{b}}$ and bond damping moment $\boldsymbol{M}_{\mathrm{d}}^{\mathrm{b}}$ (based on Eqs.(9)-(12)) are added to account for the energy dissipation in the elastic wave propagation through the bonds.

TWO-PARTICLE COLLISION

The collinear collision between two flexible rod-like particles was modeled as shown in Figure 1. Two particles with an aspect ratio of six were initially separated by a distance in the horizontal direction and with their major axes perpendicular to each other. An initial velocity was specified to the particle on the left hand side to collide with the particle on the right hand side. The interparticle friction coefficient is set to zero. During the contact process, unlike rigid particles, the flexible particles exhibited significant bending deformation, generating potential energy. After the collision, the two particles bounced apart, and translated in the horizontal direction with significant bending vibration. If bond damping was present, the particle vibration was gradually damped.

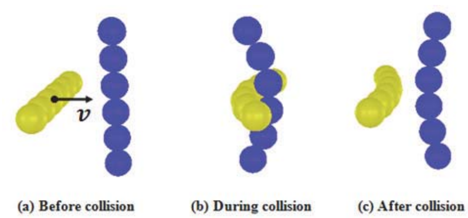


FIGURE 1. Snapshots of collinear collision between two flexible particles arranged with two major axes perpendicular to each other. An initial velocity is specified to the particle on the left hand side.

The total mechanical energy of a flexible particle is a sum of kinetic energy and potential energy. The kinetic energy can be decomposed into global kinetic energy and local kinetic energy,

$$E_{\mathrm{kin}} = E_{\mathrm{kin}}^{\mathrm{glo}} + E_{\mathrm{kin}}^{\mathrm{loc}}\,, \tag{13}$$

in which, the global kinetic energy is given by the total mass of the flexible particle, m_{p}, and the translational velocity of the center of the mass of the composite particle, v_{O}, as,

$$E_{\mathrm{kin}}^{\mathrm{glo}} = \frac{1}{2} m_{\mathrm{p}} v_{\mathrm{O}}^2\,, \tag{14}$$

and the local kinetic energy, which describes the kinetic energy relative to the center of the mass of the particle, is given by,

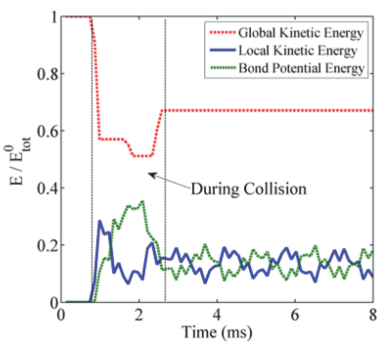
$$E_{\mathrm{kin}}^{\mathrm{loc}} = \frac{1}{2}\sum_{i=1}^{n} m_{si}(v_{si}^{r})^2 + \frac{1}{2}\sum_{i=1}^{n} J_{si}(\omega_{si})^2 \,, \quad (15)$$

where, n is the number of constituent spheres in a composite particle, v_{si}^{r} is the relative velocity of the constituent sphere i of mass m_{si} to the center of mass of the composite particle, and J_{si} and ω_{si} are the moment of inertia and angular velocity, respectively, of the constituent sphere i. Based on Eqs.(14) and (15), the global kinetic energy accounts for the kinetic energy due to the translation of the whole particle, and the local kinetic energy accounts for the kinetic energy due to particle rotation and vibration.

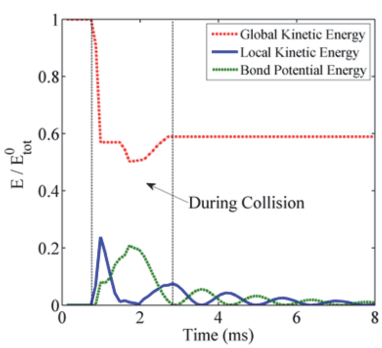
The potential energy is induced by the bond deformation and can be expressed as

$$\mathrm{E_{pot}} = \sum_{\mathrm{i=1}}^{\mathrm{n_b}} \left[\frac{1}{2}\frac{\mathrm{EA}}{\mathrm{l_b}}(\delta_{\mathrm{ni}}^{\mathrm{r}})^2 + \frac{1}{2}\frac{\mathrm{GA}}{\mathrm{l_b}}(\delta_{\mathrm{ti}}^{\mathrm{r}})^2 + \frac{1}{2}\frac{\mathrm{GI_p}}{\mathrm{l_b}}(\theta_{\mathrm{ni}}^{\mathrm{r}})^2 + \frac{1}{2}\frac{\mathrm{EI}}{\mathrm{l_b}}(\theta_{\mathrm{ti}}^{\mathrm{r}})^2\right] \quad (16)$$

in which, $\mathrm{n_b}$ is the number of bonds in a composite particle.



(a) Collision without bond damping($\beta_b = 0$)



(b) Collision with bond damping ($\beta_b = 0.676$)

FIGURE 2. Time history of various energies per particle, normalized by the initial total energy per particle, for two-particle collisions without bond damping (a) and with bond damping (b).

The time history of various energies per particle, normalized by the initial total energy per particle, $\mathrm{E_{tot}^0}$, for two-particle collisions with and without bond damping is shown in Figure 2. During collision, the global kinetic energy is partially converted to local kinetic energy and bond potential energy. After collision in the absence of bond damping, the global kinetic energy remains constant with time, and local kinetic energy and bond potential energy are constantly converted to each other. After collision with bond damping, the global kinetic energy also remains constant, while the local kinetic energy and bond potential energy are gradually damped.

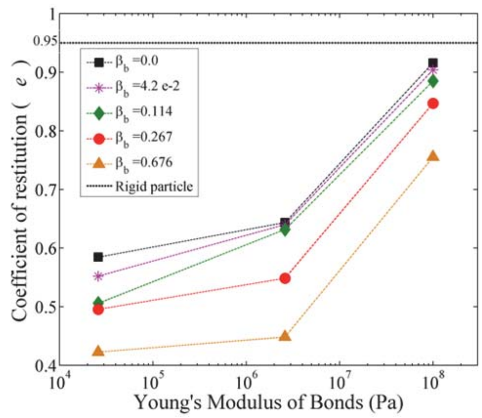


FIGURE 3. Coefficient of restitution as a function of Young's modulus of bonds for various bond damping coefficients.

The coefficient of restitution is defined as the ratio of post-collisional relative velocity to the pre-collisional relative velocity between the centers of mass of two particles. Simulations of two-particle collisions, as shown in Figure 1, have been performed to determine the effects of bond Young's modulus and bond damping on the coefficient of restitution. The coefficient of restitution is plotted in Figure 3 as a function of bond Young's modulus for various bond damping coefficients. The coefficient of restitution for the rigid particle contact is equal to 0.95, less than unity, due to the contact damping (Eqs.(7) and (8)). The same contact damping coefficient β_{c} was also used for all the flexible particles. Compared to the rigid particles that have infinite bond stiffness, smaller coefficients of restitution are obtained for the flexible particles. As the bond Young's modulus increases or the particles become stiffer, smaller bending deformation and shorter contact duration are obtained. Therefore, less kinetic energy is converted to potential energy with larger bond Young's modulus, leading to higher coefficient of restitution. As the bond damping coefficient increases, the coefficient of restitution is reduced due to the increase in the energy dissipation rate.

GRANULAR SHEAR FLOW

Granular shear flow of flexible rod-like particles was simulated, as shown in Figure 4. A number of frictionless flexible particles with an aspect ratio of six were randomly generated in the rectangular shear zone. In this simulation, the solid volume fraction in the shear zone was set to 0.1. The shear flow was initiated by applying a linear x-velocity profile in the vertical direction (i.e., y-direction). The periodic boundary conditions were specified in the x and z directions, and a Lees-Edwards boundary condition was applied in the y direction. The details of the computational set-up can be found in [4].

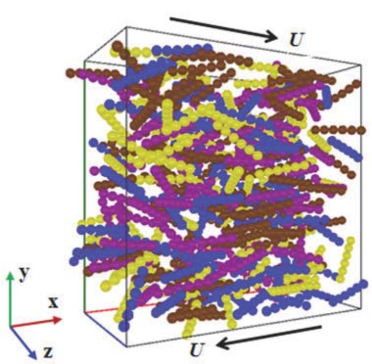


FIGURE 4. Shear flow of flexible rod-like particles at the solid volume fraction of 0.1 without gravity and fluid media.

The particle phase stress can be expressed as a sum of kinetic and collisional stresses, as defined in [5]. Figure 5 shows the normalized shear stress as a function of bond Young's modulus for shear flows with various bond damping coefficients, in which ρ_p is particle density, d_v is equivalent volume diameter of the composite particle, and γ is shear rate. In general, smaller shear stresses are obtained for shear flows with the flexible particles compared to with rigid particles. For dilute shear flows at the solid volume fraction of 0.1, the shear stress increases as the bond Young's modulus increases and decreases as the bond damping coefficient increases. The trends of the shear stress varying with bond Young's modulus and bond damping are similar to those of the coefficient of restitution (Figure 3). In conclusion, the bond properties (Young's modulus and damping) have an impact on the conversion of kinetic energy to potential energy and the dissipation rate of energies, therefore the coefficient of restitution and particle phase stress for granular shear flows are affected.

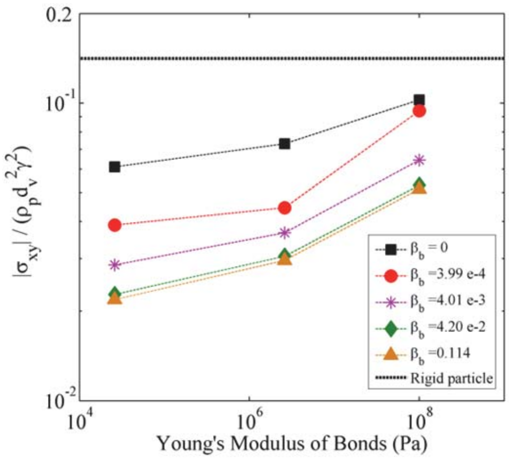


FIGURE 5. Normalized shear stress as a function of Young's modulus of bonds for shear flows of flexible rod-like particles with various bond damping coefficients. (Solid volume fraction = 0.1)

CONCLUSIONS

In the collisions between flexible particles, the kinetic energy is partially converted to potential energy, leading to a decrease in the coefficient of restitution. The bond damping can further reduce the coefficient of restitution. As a result, the particle phase stresses of granular shear flows increase as the bond stiffness increases and bond damping decreases. A comprehensive study of granular shear flows of flexible rod-like particles will be published in due course.

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