

A new kinetic theory model of granular flows that incorporates particle stiffness

Cite as: Phys. Fluids 31, 013301 (2019); doi: 10.1063/1.5051034

Submitted: 5 August 2018 • Accepted: 7 December 2018 •

Published Online: 2 January 2019



View Online



Export Citation



CrossMark

Yifei Duan^{a)} and Zhi-Gang Feng^{b)}

AFFILIATIONS

Department of Mechanical Engineering, UTSA, San Antonio, Texas 78249, USA

^{a)}Now at the Department of Chemical and Biological Engineering, Northwestern University, Illinois 60208, USA.

^{b)}Electronic mail: zhigang.feng@utsa.edu.

ABSTRACT

Granular materials of practical interest in general have finite stiffness; therefore, the particle collision is a process that takes finite time to complete. Soft-sphere Discrete Element Method (DEM) simulations suggest that there are three regimes for granular shear flows: inertial regime (or rapid flow regime), elastic regime (or quasistatic regime), and the transition regime (or elastic-inertial regime). If we use t_f to represent the mean free flight time for a particle between two consecutive collisions and t_c to represent the binary collision duration, these regimes are implicitly related to the ratio t_c/t_f . Granular flows can be successfully predicted by the classical Kinetic Theory (KT) when they are in the inertial regime of low particle-particle collision frequencies and short time contacts ($t_c/t_f \approx 0$). However, we find that KT becomes less accurate in the transition regime where the collision duration t_c is no longer small compared with the collision interval t_f ($t_c/t_f > 0.05$). To address this issue, we develop a soft-sphere KT (SSKT) model that takes particle stiffness k as an input parameter since t_c/t_f is mainly determined by k . This is achieved by proposing a modified expression for the collision frequency and introducing an elastic granular temperature T_e . Compared with the classical KT that only considers the kinetic granular temperature T_k , a redefined total granular temperature ($T_g = T_k + T_e/3$) that takes both kinetic fluctuation energy and elastic potential energy into consideration is used in the SSKT model. The model is developed for identical frictionless particles with the linear-spring-dashpot collision scheme; however, it can be extended to frictional systems as well after the modification of constitutive equations. We show that the proposed SSKT extends the applicability of the KT framework to the transition regime without losing significant accuracy. The rheological crossover has been explained physically, and the regime boundaries that separate the inertial regime and the elastic regime are quantitatively determined, showing good agreement with the previous regime map that was based on the DEM simulations. Our SSKT predictions also show that for unsteady flows such as homogeneous cooling, the particle stiffness could have a large impact on the granular flow behavior due to the energy transfer between T_e and T_k .

Published under license by AIP Publishing. <https://doi.org/10.1063/1.5051034>

I. INTRODUCTION

Continuum modeling of granular and gas-solid flows generally involves the use of Kinetic Theory (KT) models for the particle phase.^{1,2} Many KT models have been derived for dilute flows of rigid, frictionless spheres, which are the extensions of the classical kinetic theory of gases. One important difference between solid particles and gas molecules is that the kinetic energy is conserved in the elastic molecule collisions but not conserved in the inter-particle inelastic collisions. KT requires inter-particle collisions to be instantaneous, admitting of only

binary collisions, so in theory, particles have to be rigid with an infinity spring constant k .

Granular particles typically have sizes that are much larger than one hundred microns. External fields such as gravity would have a much stronger effect on granular flows, which makes it difficult to experimentally investigate the flow behavior. Instead, simulations that use Lagrangian methods to track the motion of individual particles are often used to verify the KT model without the drawback of including gravity or other external effects. In general, there are two Lagrangian methods,

depending on if particle deformation is allowed during collisions. The first one is the event-driven hard sphere (HS) method, in which the simulation time step can vary according to the collision interval and the changes in the particle velocity occur as instantaneous and discontinuous events. Multi-body contact is not allowed in the HS method, and this method may diverge at a high collision frequency, resulting in the so-called inelastic collapse.^{3,4} The second approach is the soft-sphere Discrete Element Method (DEM).⁵ In the DEM, the collision is not an instantaneous event; it is resolved with a simulation time step that is much smaller than the collision duration. Both normal and tangential interactions in the DEM could be implemented by modeling the deformations of the particles; other effects such as cohesive and repulsive forces could also be added. Most importantly, the DEM allows multi-body collisions and it is more effective for granular flows in the regime where collisions take place frequently. Similar to the DEM, there is another method called Contact Dynamics (CD). It uses an implicit scheme that allows larger simulation time steps and a nonsmooth formulation to solve particle dynamics.^{6,7}

When it comes to a granular system of practical interest, particles always have finite stiffness. This means that the collision is a process that takes finite time to complete and the collision duration could be comparable to the collision interval at a high collision frequency. Granular flows in this case can be very complex. Based on the DEM simulations of homogeneous shear flow, it was observed that granular flows could show either fluid-like behavior or solid-like behavior. In the early modeling work, generally two regimes are distinguished: inertial regime (or rapid-flow regime) and elastic regime (or quasi-static regime).⁸ The difference of flow behavior between elastic and inertial regimes can be attributed to the micro-scale phenomena at the particle level. In the inertial regime, the collision duration is negligible compared to the collision interval and the hydrodynamic behaviors of granular flows are mainly dominated by the rapid binary collisions. Many researchers have reported that the instantaneous binary collision assumption is still valid even for relatively dense flows if the stiffness of contacts between particles is sufficiently large;⁹⁻¹¹ flows in this case can still be considered in the inertial regime. Despite the existence of velocity correlation for dense flows that could affect the KT predictions,^{10,12} classical KT exhibits generally good agreement with DEM simulation results.¹³ However, in the elastic flow regime, many adjacent particles are engaged in filament-like clusters that are called force chains; the collision duration becomes comparable to the collision interval and the sustained multi-particle contacts start to prevail. With elastic flows being dominated by enduring and multi-particle contacts, the collision duration can no longer be ignored. In the elastic regime, the stress is observed to be independent of the shear rate since the transport can occur between particles through the elastic waves traveling across the contact points at a rate which is governed by the elastic properties and not by the granular temperature.¹⁴

The transition between these regimes is observed to be smooth, which suggests that purely elastic or inertial flows

are achieved only within certain limits.¹⁵ Many researchers constructed regime maps to better understand the regime transition. The transition regime or the so-called elastic-inertial regime is identified for a stress scale using both elastic and inertial properties. Campbell¹⁴ presented his regime map based on a series of DEM simulations of homogeneous shear flow including cases that are near the elastic limit. He adopted the dimensionless group $k/\rho d^3 \dot{\gamma}^2$ to help understand the rheology of the granular materials. Here, ρ is the particle density, d is the particle diameter, k is the particle stiffness, and $\dot{\gamma}$ is the shear rate. In general, the value of $k/\rho d^3 \dot{\gamma}^2$ reflects the ratio of the relative effects of the elastic contribution to the collisional contribution; the collisional effect dominates when $k/\rho d^3 \dot{\gamma}^2$ is large. As the shear rate increases, both elastic and inertial regimes approach the intermediate or transition regime that shows a stress scaling $\dot{\gamma}^a$ with $0 < a < 2$. As the name suggests, the flows in the transition regime show mixed characteristics of both elastic flows and inertial flows. This is different from the elastic regime where $\tau \propto \dot{\gamma}^0$ or the inertial regime where $\tau \propto \dot{\gamma}^2$. Classical KT fails to predict the hydrodynamic behavior of granular flows in the transition regime. To model granular flows in the transition regime, researchers came up with an approach that is based on the dimensional analysis to identify dimensionless parameters of the problem. The solution of this approach is the algebraic relations between those parameters, and this approach is called $\mu(I)$ rheology.¹⁶

In the context of $\mu(I)$ rheology, there are two dimensionless numbers to characterize the granular flow regimes. One is the inertial number $I = \dot{\gamma}d/\sqrt{P/\rho}$, and the other is the contact stiffness number $\kappa = k/Pd$. I indicates the ratio of inertial forces to the normal pressure P , and κ compares the elastic force to the normal pressure P . Consider that in the framework of $\mu(I)$ rheology, the solid volume fraction ϕ does not change, and $\kappa/I^2 = k/\rho d^3 \dot{\gamma}^2$. These two dimensionless numbers I and κ are equivalent to ϕ and $k/\rho d^3 \dot{\gamma}^2$ from the work of Campbell. Both sets of dimensionless numbers can describe the granular flow regimes, and they are complementary; they are obtained from two different types of simulations: one is the pressure controlled shearing, and the other is the volume controlled shearing. However, the contact stiffness is often assumed to be very large in $\mu(I)$ rheology by only focusing on the cases that have $\kappa > 10^4$.¹⁶ At a large contact stiffness number κ , the effect of particle stiffness is simplified and the inertial number I becomes the only parameter that characterizes the flow regimes. A large value of I corresponds to the inertial regime, while small I corresponds to the elastic regime. The $\mu(I)$ model has been proved to be valuable in terms of modeling “liquid-like” granular flows.¹⁷⁻¹⁹ However, without considering κ , the simplified $\mu(I)$ model cannot cover a wide range of granular flows as described in the work by Campbell.¹⁴ It is ill-posed for both high and low inertial numbers as enduring elastic force chains and binary collisions becomes important at these limits and the dimensionless analysis fails to consider the additional physics during regime transition.²⁰ The rheology that can transition seamlessly between different regimes remains a challenge.

The aim of the present work is to extend the classical KT and develop a new KT model that can capture the mixed behavior of granular flows in the transition regime. Most of the existing KT models are limited to granular flows near the inertial limit. There are primarily three factors that could affect the accuracy of these KT models as granular flows move away from the inertial limit: the reduced energy dissipation rate due to the existence of velocity correlation for dense granular shear flows, the reduced collision frequency as a result of the finite particle contact duration, and the non-dissipative elastic potential energy that is caused by particle collisional deformation. Among these three factors, the first one is the consequence of particle contact inelasticity and the last two stem from the breakdown of an instantaneous collision assumption due to the finite stiffness of particles. The velocity correlation factor has been well studied, and it is believed to be the main factor that causes the discrepancy between the KT predictions and the DEM simulation results for dense homogeneous shear flows.^{21,22} Berzi and Jenkins²³ studied how the particle contact duration could reduce the collision frequency of soft-sphere granular systems and affect the collisional terms. They adjusted the granular temperature of homogeneous shear flows to account for velocity correlations. They have shown that for shear flows, their model is able to produce results that agree well with the DEM simulations. However, the effect of particle stiffness to the transfer between the particle kinetic energy and elastic potential energy has not been considered in the KT models although this factor is well known in the DEM simulations.²⁴⁻²⁶

In the context of classical KT, kinetic granular temperature T_k , expressed as the average kinetic fluctuating energy, is defined to describe the collisional behavior due to particle movement,

$$T_k = \frac{1}{3N} \sum_{i=1}^N (\mathbf{c}_i - \mathbf{u})^2, \quad (1)$$

where N is the number of particles in a system, \mathbf{c} is the individual particle's velocity, and \mathbf{u} is the local average velocity. Since no particle deformation is considered in the classical KT models, the granular temperature T_g defined in these models is equivalent to the kinetic granular temperature T_k defined in this work. The measured "granular temperature" from DEM simulations in the literature is calculated from Eq. (1), which is referred as T_k here. The lack of a second parameter to model the elastic behavior of particle deformation makes many KT models inappropriate for soft-sphere systems in the transition regime.

In this study, we develop a soft-sphere KT (SSKT) model that relaxes the instantaneous collision assumption. We show that the SSKT can extend the applicability of the classical KT to the transition regime without losing significant accuracy. This is achieved by the incorporation of two modifications in the SSKT model. The first one is to include the particle stiffness by introducing an elastic granular temperature T_e that signifies the amount of elastic potential energy in the system. Similar

to the definition of kinetic granular temperature, we define the elastic granular temperature as

$$T_e = \frac{1}{mN} \sum_{i=1}^{N_{col}} k_n \xi_i^2, \quad (2)$$

where N_{col} is the average number of contacts in a system, m is the mass of the particle, k_n is the normal stiffness, and ξ_i is the particle overlap of the i th collision. An analytical solution to the elastic granular temperature is obtained that can be calculated using the ratio of particle collision time to mean flight time, t_c/t_f , which is explicitly related to the particle stiffness. In the inertial regime where $t_c/t_f \approx 0$, we have $T_e \approx 0$ and $T_g \approx T_k$, and the SSKT model is reduced to the classical KT model. As t_c/t_f increases, there would be a significant amount of energy which exists in the form of non-dissipative elastic potential energy, and we define the granular temperature $T_g = T_k + T_e/3$. The hydrodynamic behavior of granular flow is determined by the particle velocity distribution, which is a function of T_k instead of T_g . The SSKT model has better prediction due to its ability to differentiate T_k from T_g at large t_c/t_f . The second modification is similar to the one proposed by Berzi and Jenkins.²³ The constitutive relations are modified to reflect the reduced collision frequency as a result of the finite collision duration. A new correlation is developed for the particle collision frequency that includes the effect of the solid volume fraction; this correlation can be extended to dense granular flows. The collisional terms such as pressure and shear stress are modified using this new correlation, and the results are validated by the DEM simulations. We then apply the SSKT model to study the free cooling process and simple shear flows. We find that the SSKT model is not only able to explain the discrepancy between the DEM simulation results and the predictions of classical KT but also able to produce results that agree well with the DEM simulations. Furthermore, instead of constructing a regime map based on the DEM simulation data, we create a new type of regime map based on the ratio of the elastic potential energy to the kinetic fluctuation energy.

II. THE SOFT-SPHERE KINETIC THEORY MODEL

Application of any KT model involves the kinetic equation for the particle velocity distribution function. The single-particle velocity distribution function $f(\mathbf{c}, \mathbf{r}, t)$ governs the macroscopic properties of solid particles, which is a function of granular temperature. Here \mathbf{c} , \mathbf{r} , and t are the particle velocity, position vector, and time variable, respectively. There are two granular temperatures defined in this work. Kinetic granular temperature T_k corresponds to the particle fluctuations, while elastic granular temperature T_e corresponds to the particle deformation. The classical KT model is for rigid body hard-sphere systems; it has no particle deformation, so $T_g = T_k$ for these systems. The granular temperature for hard-sphere systems can refer to either T_g or T_k since they are equal. However, for soft-sphere systems, T_k is not equal to T_g and the single particle velocity distribution function $f(\mathbf{c}, \mathbf{r}, t)$ is determined by T_k instead of T_g .

For dilute homogeneous shear flows under uniform shear $\dot{\gamma}$ without an external effect, we can write the kinetic fluctuation energy balance equation as

$$\frac{3}{2}\rho\phi\frac{dT_g}{dt} = \tau\dot{\gamma} - \Gamma, \tag{3}$$

where τ is the shear stress, and Γ is the energy dissipation rate. A complete energy balance equation for general cases and the related transport coefficients can be found in Ref. 27. By defining the total granular temperature $T_g = T_k + T_e/3$ on the left-hand side of the equation, it can capture the energy transfer between kinetic energy and elastic potential energy observed in the DEM simulations. If we can express T_e as a function of T_k , the energy balance equation can be closed and the change in T_k is a result of both inelastic collision and the energy transfer from or to T_e .

Based on the averaging method,²⁸ Artoni and Richard²⁹ derived the balance equations to consider the conversion of mechanical energy due to affine deformations. Although they did not directly include the elastic energy in the energy balance equation, an additional energy dissipation term was introduced for the long-lasting contacts. Kondic and Behringer²⁴ explored the role of elasticity in a system and showed that the elastic energy could be larger than the kinetic fluctuation energy in cases of a high solid volume fraction. This portion of energy, T_e , cannot be dissipated during collisions, but it can be transferred to T_k spontaneously, which will eventually affect the bulk behavior of granular flows. In this section, we derive a model based on the linear-spring-dashpot (LSD) scheme in order to calculate the amount of elastic energy in a system. The LSD model is commonly used to calculate the inelastic force between colliding spheres in the DEM simulations. It leads to a constant coefficient of normal restitution. For the collision of two identical frictionless particles, the particle normal interaction during a contact is described as follows:

$$\ddot{\xi} = -\frac{k}{m_{eff}}\xi - \frac{\eta_n}{m_{eff}}\dot{\xi}, \tag{4}$$

where $m_{eff} = m/2$, m is the mass of the particle, η_n is the normal damping coefficient, and ξ is the normal overlap of two colliding particles. By solving Eq. (4) with the initial conditions of $\xi = 0$ and $\dot{\xi} = V$, we have

$$\xi = \frac{V}{\sqrt{1-\beta^2}\omega_0} \sin\left(\sqrt{1-\beta^2}\omega_0 t\right) \exp(-\beta\omega_0 t), \tag{5}$$

$$\begin{aligned} \dot{\xi} = & V \cos\left(\sqrt{1-\beta^2}\omega_0 t\right) \exp(-\beta\omega_0 t) - \frac{V\beta}{\sqrt{1-\beta^2}} \\ & \times \sin\left(\sqrt{1-\beta^2}\omega_0 t\right) \exp(-\beta\omega_0 t). \end{aligned} \tag{6}$$

Here, $\beta = \frac{\eta_n}{2\sqrt{k_n m_{eff}}}$, $\omega_0 = \sqrt{\frac{k_n}{m_{eff}}}$, and V is the pre-collision normal relative velocity at the point of contact. Given the value of the normal restitution coefficient e , the normal damping coefficient and binary collision duration can then be obtained,

$$\eta_n = \frac{2\sqrt{m_{eff}k_n}|\ln e|}{\sqrt{\pi^2 + \ln^2 e}}, \tag{7}$$

$$t_c = \pi \left(\frac{k_n}{m_{eff}} - \frac{\eta_n^2}{4m_{eff}^2} \right)^{-\frac{1}{2}}. \tag{8}$$

At any given time, the total elastic energy in the system is measured by

$$E_e = \frac{1}{2} \sum_{i=1}^{N_{col}} k_n \xi_i^2, \tag{9}$$

where N_{col} is the total number of collisions at this specific time and ξ_i is the overlap of i th collision in the system. The time averaged square of the normal overlap $\overline{\xi_i^2}$ during i th collision follows

$$\overline{\xi_i^2} = \frac{1}{t_c} \int_0^{t_c} \xi_i^2 dt = \frac{1}{2} \left(\frac{V_i}{\omega_0} \right)^2 \left[1 - \frac{\sqrt{1-\beta^2} \sin\left(\frac{2\pi}{\sqrt{1-\beta^2}}\right)}{2\pi} \right]. \tag{10}$$

Here, V_i is the pre-collision normal relative velocity component at the point of contact of i th collision. Substituting $\omega_0 = \sqrt{\frac{2k_n}{m}}$ into Eq. (10), we have

$$k_n \overline{\xi_i^2} = \frac{1}{4} m V_i^2 \left[1 - \frac{\sqrt{1-\beta^2} \sin\left(\frac{2\pi}{\sqrt{1-\beta^2}}\right)}{2\pi} \right]. \tag{11}$$

For a soft-sphere system with large portion of elastic potential energy, there are a lot of collisions taking place in the system, so the sum of ξ_i^2 of each collision at any given time could be approximated by the sum of the time averaged value $\overline{\xi_i^2}$,

$$\sum_{i=1}^{N_{col}} \xi_i^2 \approx \sum_{i=1}^{N_{col}} \overline{\xi_i^2}. \tag{12}$$

Then we can rewrite Eq. (2) based on Eqs. (11) and (12) as

$$T_e = \frac{\sum_{i=1}^{N_{col}} (k_n \overline{\xi_i^2})}{mN} = \frac{1}{4} \frac{N_{col}}{N} V_{avg}^2 \left[1 - \frac{\sqrt{1-\beta^2} \sin\left(\frac{2\pi}{\sqrt{1-\beta^2}}\right)}{2\pi} \right], \tag{13}$$

where $V_{avg}^2 = \frac{1}{N_{col}} \sum_{i=1}^{N_{col}} V_i^2$. According to the KT, for three dimensional systems, the energy dissipation rate is³⁰

$$\Gamma = \frac{12\rho\phi^2(1-e^2)g_0 T_k^{\frac{3}{2}}}{d\sqrt{\pi}}, \tag{14}$$

where e is the coefficient of restitution, and g_0 is the radial distribution function.³¹ We assume that only binary collisions exist in the system. The collision frequency per particle is equal to the inverse of mean free flight time between two consecutive collisions,³²

$$t_f^{-1} = \frac{12}{d} \phi g_0 \sqrt{\frac{T_k}{\pi}}. \tag{15}$$

t_f^{-1} can be interpreted as the average number of collisions per second for each individual particle. The derivation of Eq. (15) can be found in the Appendix. Within one second, the total number of collisions in the system is Nt_f^{-1} . Γ is defined as the energy dissipation per second, so the average energy dissipation per collision is as follows:

$$\frac{\Gamma}{Nt_f^{-1}} = m(1 - e^2)\Gamma_k. \tag{16}$$

The average kinetic energy change during a collision could also be derived based on the restitution coefficient as follows:

$$\frac{1}{N_{col}} \sum_{i=1}^{N_{col}} \Delta E_i = \frac{1}{4}m(1 - e^2)V_{avg}^2. \tag{17}$$

$\Delta E_i = \frac{1}{4}m(1 - e^2)V_i^2$ is the transnational kinetic energy change during a collision.¹ Since both expressions on the right-hand side of Eqs. (16) and (17) are the energy dissipation per collision and they must be equal, we can relate the average normal collision velocity V_{avg} to the kinetic granular temperature T_k by

$$V_{avg}^2 = 4T_k. \tag{18}$$

By combining Eqs. (13) and (18), the ratio of elastic temperature to kinetic temperature can be written by

$$\frac{T_e}{T_k} = \frac{N_{col}}{N} \left[1 - \frac{\sqrt{1 - \beta^2} \sin\left(\frac{2\pi}{\sqrt{1 - \beta^2}}\right)}{2\pi} \right]. \tag{19}$$

To verify Eq. (19), we calculate the value of $NT_e/N_{col}T_k$ from the DEM simulations. The DEM simulations were performed using the MFIX package,³³ which is available from the National Energy Technology Laboratory (NETL). The DEM simulation time step Δt must be sufficiently small compared with the particle collision time t_c in order to resolve the particle collision process. For the present simulations, we chose $\Delta t = t_c/50$, a practice successfully employed by others.^{21,34,35} Particles were packed into a cubic domain with periodic boundaries. Each particle was given an initial velocity that follows the Maxwell distribution function, so the system has an initial granular temperature $T_g = T_k$. We choose $e = 1$ so that without external effects, the total energy in the system remain constant and the system quickly reaches a steady state. At a steady state, T_e becomes a non-zero term and $T_g = T_k + T_e$. Both T_e and T_k can be calculated from DEM simulations based on their definitions.

According to Eq. (19), the ratio $NT_e/N_{col}T_k$ is only related to the particle properties and it is close to 1 if the normal restitution coefficient $e \rightarrow 1$. We calculated the ratio from DEM simulations of granular flows with $e = 1$ at different granular temperatures and found good agreement with Eq. (19), as shown in Fig. 1. Note that the derivation is not limited to $e = 1$ or a steady state although a rapid change in T_e can slightly affect the accuracy of Eq. (12). The relation between T_k and T_e is still valid at $e < 1$, which can be proved in the homogenous cooling case in Sec. III B.

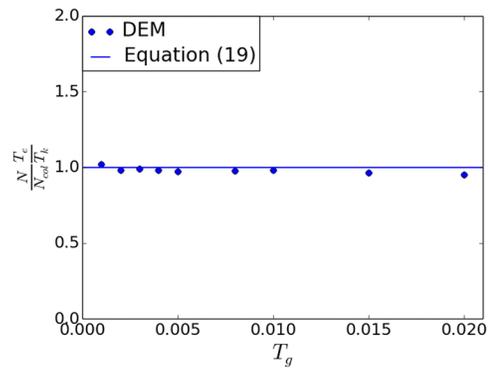


FIG. 1. $NT_e/N_{col}T_k$ at different initial granular temperature T_g in m^2/s^2 . Simulations were set up in a cubic domain using 2984 particles with periodic boundary conditions ($\phi = 0.2$). Dots represent the time averaged ratio from the DEM simulations.

Since a collision is a process that takes a finite amount of time t_c to complete, particle is considered in a collision state during this time window of t_c . If the mean free flight time of each particle is t_f , the probability of any particle in the collision state will be t_c/t_f , so we expect $N_{col}/N = t_c/t_f$ at any given time. Therefore, we can rewrite Eq. (19) to

$$T_e = t_c t_f^{-1} \left[1 - \frac{\sqrt{1 - \beta^2} \sin\left(\frac{2\pi}{\sqrt{1 - \beta^2}}\right)}{2\pi} \right] T_k. \tag{20}$$

To verify Eq. (20), DEM simulations were performed to compute the value of T_e/T_k of the system. Initial particle velocities were given based on the initial granular temperature T_g ; the values of T_e/T_k were calculated as a function of time. From Fig. 2(a), we can see that for a system with particles of finite stiffness, our proposed model could predict the ratio of T_e to T_k that matches the DEM results very well. However, it starts to deteriorate as the portion of elastic energy further increases. This is because the model relies on the velocity profile that is based on the binary collision assumption. It is expected that with the increasing portion of non-binary collisions, the proposed model would become less accurate and the time averaged elastic deformation becomes more complicated. Based on the probability analysis, the binary collision percentage in a system is^{4,32}

$$P_{binary} = \exp(-2t_c t_f^{-1}). \tag{21}$$

T_e/T_k is shown to increase with t_c/t_f , as shown in Fig. 2(b). From Fig. 3, we find that a larger T_e/T_k results in a larger fraction of non-binary collisions, which reduces the accuracy of our proposed models. This is evidenced in Fig. 2(b). For a DEM simulation with $t_c/t_f = 0.4$, the proposed model can still predict the ratio of T_e to T_k quite well with less than 10% difference compared to the DEM simulation results. In other word, the non-binary collisions which weight about 65% of the total collisions in the DEM simulations cause only

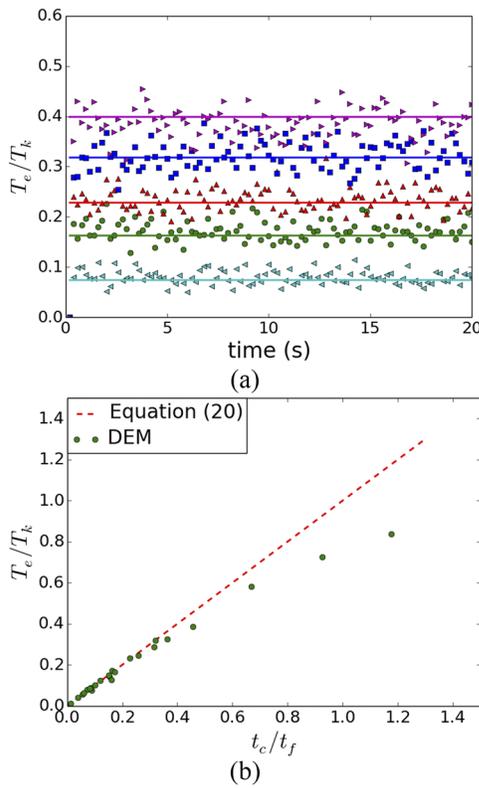


FIG. 2. T_e/T_k compared with DEM results at different t_c/t_f . (a) The ratio of the elastic temperature T_e to the kinetic temperature T_k in granular systems with different t_c/t_f . Markers represents the DEM results (from top to bottom, $t_c/t_f = 0.07, 0.16, 0.22, 0.30, 0.38$), and lines are the predictions from Eq. (20). (b) The value of T_e/T_k along with the ratio of binary collision time to collision interval t_c/t_f . The dashed line indicates the theoretical prediction; dots represent DEM results at ϕ ranging from 0.1 to 0.5.

10% difference compared with the ideal case of all binary collisions.

When it comes to the SSKT model, the single-particle velocity distribution function should be determined by T_k instead of T_g ; the existence of elastic energy should affect the fluctuation energy dissipation rate since this portion of energy could not be dissipated during collisions, but it could be transformed into the form of kinetic energy at any time. This introduces one more unknown T_k , and Eq. (20) has to be used as a closed-form constitutive expression.

Moreover, we found that with the increase in t_c/t_f , the actual collision frequency is less than the value predicted by the classical KT,

$$f_{KT} = \frac{12}{d} \phi g_0 \sqrt{\frac{T_k}{\pi}}. \quad (22)$$

Equation (22) represents the KT prediction of the collision frequency for hard sphere systems; it yields good agreement with the hard sphere simulation results.³² As shown in Fig. 4, we find that the collision frequency for soft sphere systems

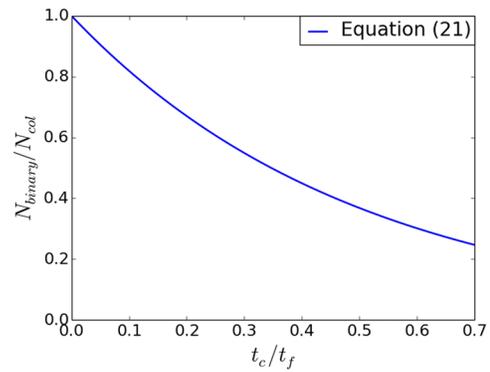


FIG. 3. The ratio of the number of binary collisions to the number of total collisions in a system.

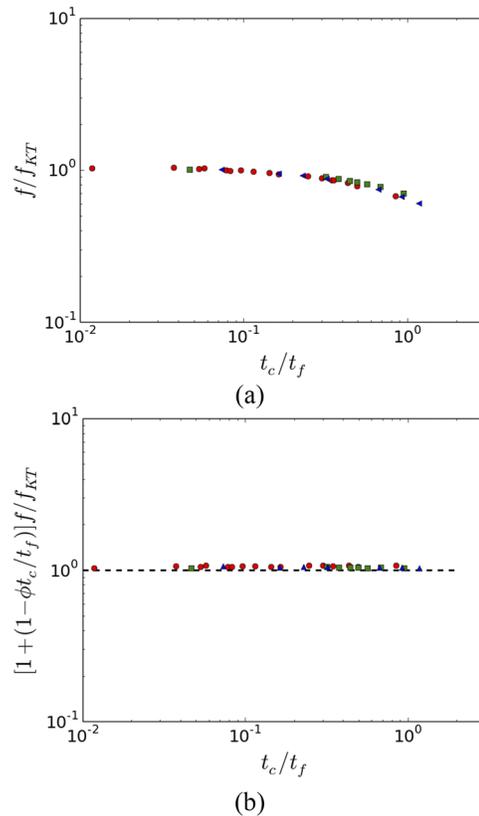


FIG. 4. Markers represent DEM results (circles: $\phi = 0.3$; triangles: $\phi = 0.4$; and squares: $\phi = 0.5$). (a) The ratio of the measured collision frequency f from DEM to the predicted collision frequency f_{KT} by classical KT for granular systems at different t_c/t_f . (b) Rescaled ratio $[1 + (1 - \phi)t_c/t_f]f/f_{KT}$ at different t_c/t_f .

decreases when t_c/t_f increases. Based on the DEM simulation results, we found that the soft sphere collision frequency could be nicely correlated by the following equation:

$$f = \frac{f_{KT}}{1 + (1 - \phi)t_c/t_f}. \tag{23}$$

This expression resembles the one proposed by Berzi and Jenkins,²³ $f = \frac{f_{KT}}{1+t_c/t_f}$, when the system is extremely dilute (i.e., $\phi \approx 0$). Because the collisional stress and dissipation rate of kinetic fluctuation energy are proportional to the collision frequency, the constitutive relations that are derived for hard spheres should be modified accordingly in order to be used for soft spheres. Based on the expressions of the kinetic theory for hard spheres,^{36,37} the constitutive equations of the SSKT model are listed in Table I. The expressions for classical KT and the extended KT by Berzi and Jenkins²³ are also listed for comparison.

In Table I, the energy dissipation rate Γ of classical KT can be found in many KT models,^{1,37} and the pressure p and shear stress τ of classical KT are obtained from Eqs. (25) and (26) in the work by Berzi and Jenkins.²³ Note that if we use p_{KT} to represent the prediction of classical KT, the modified pressure is written as $p^{-1} = p_{KT}^{-1} + (p_{KT} \frac{t_c}{t_f})^{-1}$ in their extended KT model. This is equivalent to the modification that all collision frequency related terms are multiplied by a factor f/f_{KT} or $1/(1 + t_c/t_f)$, which is the form we used in Table I. As an intermediate variable, the collision frequency f_{KT} is not explicitly derived in many KT models, and its definition may vary case by case. In our work, f_{KT} is defined as the number of collisions per particle in 1 s. The detailed derivation can be found in the Appendix. Also the expression of T_e from SSKT in Table I has a different form compared with Eq. (20), in which K and H are used to replace t_c/t_f ($t_c/t_f = KT_k^{1/2}$), so T_k can be moved to the right-hand side of the equation. Due to the reduced collision

frequency, terms that are derived based on particle collisions are multiplied by f/f_{KT} according to Eq. (23).

To validate the proposed SSKT model, we compared the predicted collision frequency with the DEM simulation results. We performed several DEM simulations with different t_c/t_f at $\phi = 0.3$. Our results were compared with the predictions from the model by Berzi and Jenkins²³ based on measured T_k from DEM. As shown in Fig. 5(a), the collision frequency predicted by the SSKT model could match the reduced collision frequency better as t_c/t_f increases. In general, the flow pressure could be divided into two parts, $p = p_{col} + p_{kin}$. Here, p_{col} is related to the collision frequency and p_{kin} is related to the particle kinetic fluctuation. The SSKT predicts that p_{kin} is not affected by the elastic energy and p_{col} varies along with the reduced collision frequency, as shown in Fig. 5(b).

In the case of steady shear flows, the driving forces are converted to granular temperature through shear work, and “heat” is dissipated through inelastic collisions. For dense steady-state shear flows, the velocity correlation as a result of the force chain has to be considered,^{38,39}

$$\Gamma \frac{d}{L} = \tau \dot{\gamma}, \tag{24}$$

$$L = \max \left[\frac{2(1-e)}{15} (g_0 - g_{0,f}) + 1, 1 \right]. \tag{25}$$

Here L is the correlation length which is a function of the solid volume fraction and restitution coefficient. $g_{0,f}$ is the value of radial distribution function at $\phi_f = 0.49$.⁴⁰

Equation (24) can be further simplified and lead to $T_k \propto \dot{\gamma}^2$. We can show that for steady homogeneous shear flows,

TABLE I. Summary of model equations.

Classical KT ^{23,37}	Berzi and Jenkins ²³	SSKT
$T_g = T_k$	$T_g = T_k$	$T_g = T_k + \frac{1}{3} T_e$
$T_e = 0$	$T_e = 0$	$T_e = KHT_k^{3/2}$
$\Gamma = \frac{12}{d\sqrt{\pi}} \rho \phi^2 g_0 (1 - e^2) T_k^{3/2}$	$\Gamma = \frac{12}{d\sqrt{\pi}} \rho \phi^2 g_0 (1 - e^2) T_k^{3/2} \frac{f}{f_{KT}}$	$\Gamma = \frac{12}{d\sqrt{\pi}} \rho \phi_0^2 g_0 (1 - e^2) T_k^{3/2} \frac{f}{f_{KT}}$
$p = \rho \phi T_k + 2\rho(1 + e)\phi^2 g_0 T_k$	$p = \rho \phi T_k + 2\rho(1 + e)\phi^2 g_0 T_k \frac{f}{f_{KT}}$	$p = \rho \phi T_k + 2\rho(1 + e)\phi^2 g_0 T_k \frac{f}{f_{KT}}$
$\tau = \frac{8}{5} \rho d \phi^2 g_0 J \sqrt{\frac{T_k}{\pi}} \dot{\gamma}$	$\tau = \frac{8}{5} \rho d \phi^2 g_0 J \sqrt{\frac{T_k}{\pi}} \dot{\gamma} \frac{f}{f_{KT}}$	$\tau = \frac{8}{5} \rho d \phi^2 g_0 J \sqrt{\frac{T_k}{\pi}} \dot{\gamma} \frac{f}{f_{KT}}$
$f_{KT} = t_f^{-1} = \frac{12}{d} \phi g_0 \sqrt{\frac{T_k}{\pi}}$	$f_{KT} = t_f^{-1} = \frac{24}{d} \phi g_0 \sqrt{\frac{T_k}{\pi}}$	$f_{KT} = t_f^{-1} = \frac{12}{d} \phi g_0 \sqrt{\frac{T_k}{\pi}}$
$J = \frac{1+e}{2} + \frac{\pi(1+e)^2(3e-1)}{96-24(1-e)^2-20(1-e^2)}$	$J = \frac{1+e}{2} + \frac{\pi(1+e)^2(3e-1)}{96-24(1-e)^2-20(1-e^2)}$	$J = \frac{1+e}{2} + \frac{\pi(1+e)^2(3e-1)}{96-24(1-e)^2-20(1-e^2)}$
	$t_c = \frac{d}{5} \left(\frac{\rho \pi d}{4k} \right)^{\frac{1}{2}}$	$t_c = \pi \left(\frac{k_n}{m_{eff}} - \frac{\eta_n^2}{4m_{eff}^2} \right)^{-\frac{1}{2}}$
	$\frac{f}{f_{KT}} = \left[1 + \frac{t_c}{t_f} \right]^{-1}$	$\frac{f}{f_{KT}} = \left[1 + (1 - \phi) \frac{t_c}{t_f} \right]^{-1}$
		$\eta_n = \frac{2\sqrt{m_{eff} k_n} \ln e }{\sqrt{\pi^2 + \ln^2 e}}$
		$\beta = \frac{\eta_n^2}{2\sqrt{k_n m_{eff}}}$
		$K = \frac{12}{d} \phi g_0 \sqrt{\pi} \left(\frac{k}{m_{eff}} - \frac{\eta_n^2}{4m_{eff}^2} \right)^{-\frac{1}{2}}$
		$H = 1 - \frac{1}{2\pi} \sqrt{1 - \beta^2} \sin\left(\frac{2\pi}{\sqrt{1 - \beta^2}}\right)$

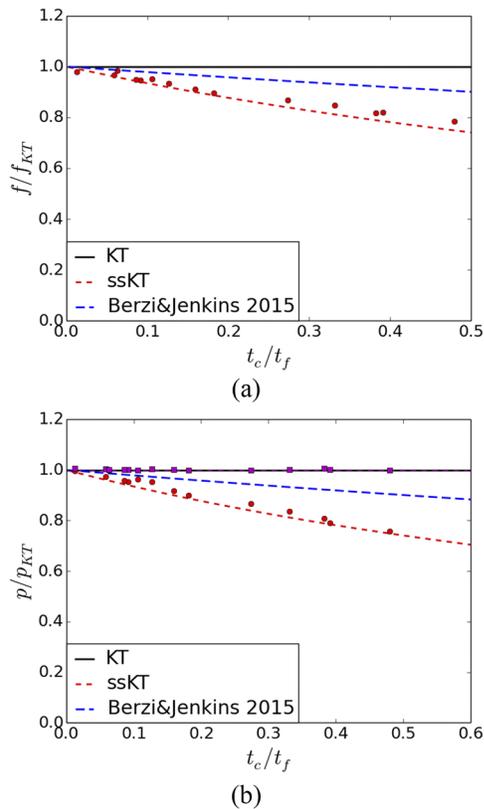


FIG. 5. Comparison between the prediction of KT models and DEM simulation results. (a) Collision frequency f (circles represent DEM results). The predicted collision frequency and pressure by Berzi and Jenkins²³ are also plotted for comparison. (b) p_{kin} and p_{col} (circles represent p_{col} , and squares represent p_{kin} from DEM results). The predicted collision frequency and pressure by Berzi and Jenkins²³ are also plotted for comparison.

T_e remains constant, which does not enter the energy balance equation. The effect of the reduced collision frequency f/f_{KT} on both sides of Eq. (24) is canceled out as well. The particle stiffness would have no impact on the bulk behavior if the flows are at a steady state and the energy diffusion is negligible. However, particle stiffness can affect the constitutive relation between stresses and kinetic granular temperature. If we let p_{hard} , τ_{hard} , and T_{hard} be the collisional pressure, shear stress, and kinetic temperature predicted by the classical KT model and let p_{soft} , τ_{soft} , and T_{soft} be the pressure, shear stress, and kinetic temperature predicted by the SSKT model, we have found $T_{soft}/T_{hard} = 1$, $p_{soft}/p_{hard} = f/f_{KT}$, $\tau_{soft}/\tau_{hard} = f/f_{KT}$, and $p_{soft}/\tau_{soft} = p_{hard}/\tau_{hard}$. Therefore, the change in particle stiffness of homogeneous shear flows will not change T_k and τ/p . This is evidenced in the DEM simulations by Vescovi and Luding⁴¹ as shown in Table II. Comparing two simple shear DEM simulations at $\phi = 0.6$ with $k/\rho d^3 \dot{\gamma}^2$ being equal to 10^3 and 10^7 , respectively, the difference between the τ/p values is less than 2% and the difference between the T_k values is less than 11%. However, the difference between the p values is as large as 75% and the

TABLE II. Measurement of steady state quantities at $\phi = 0.6$ from Vescovi and Luding.⁴¹

$k/(\rho d^3 \dot{\gamma}^2)$	$p/(\rho d^2 \dot{\gamma}^2)$	$\tau/(\rho d^2 \dot{\gamma}^2)$	$T_k/(d^2 \dot{\gamma}^2)$	τ/p
10^3	11.14	3.26	0.58	0.2926
10^7	40.48	11.85	0.66	0.2927

difference between the τ values is 72%. This shows that the particle stiffness has a significant impact on the pressure and shear stress fields of granular shear flows.

III. THE EFFECT OF PARTICLE STIFFNESS ON GRANULAR FLOWS

A. Steady shear flows and regime maps

For steady homogeneous shear flows, T_e remains constant, which does not enter the energy balance equation. Although T_e of steady shear flows has no impact on the granular flow behavior, it can be used to indicate the granular flow regime and help quantitatively determine the boundaries on the regime map. Using data obtained from DEM simulations, many researchers constructed a regime map for granular flows to better understand the regime transition. Campbell unified the various granular flow theories and filled in the gap between the elastic granular flows and rapid granular flows.¹⁴ In his theory, the ratio of the elastic effect to the inertial effect is governed by a dimensionless parameter: $k/(\rho d^3 \dot{\gamma}^2)$. Since $k/(\rho d^3 \dot{\gamma}^2) \propto 1/(\gamma t_c)^2$, this ratio can be further interpreted as the square of the ratio of $1/\gamma$, a time scale that is relevant to how quickly particles are drawn together by the shear flow and how quickly the elastic contact forces push them apart.⁴² A complete flow map for shearing granular materials was presented based on the DEM simulation results, as shown in the left column of Fig. 6. His theory leads to the ironic conclusion that rapid granular flows (i.e., granular flows in the inertial regime) occur only at small shear rates when the solid volume fraction is fixed. He explained that the increasing shear rate could compel the formation of force chains at lower concentrations. This phenomenon, on the other hand, could be explained by the SSKT model based on the role of elastic energy: the increasing shear rate could result in high temperature and high collision frequency, making the binary collision time comparable to the collision interval and invalidating the instantaneous collision assumption. The inertial-non-collisional regime on his map is equivalent to the transition regime as we discussed in this study; it indicates the limit where the KT starts to deteriorate as the elastic effect begins to dominate. The KT model becomes invalid as the flow moves further into the elastic regime. However, the transition regime on his regime map was estimated based on the DEM simulation results, and his theory did not provide an analytical method to accurately determine the extent of the elastic effect in the transition regime.

Sun, Jin, and Zhou²⁶ analyzed their DEM simulation results and found that the ratio of elastic energy to the kinetic

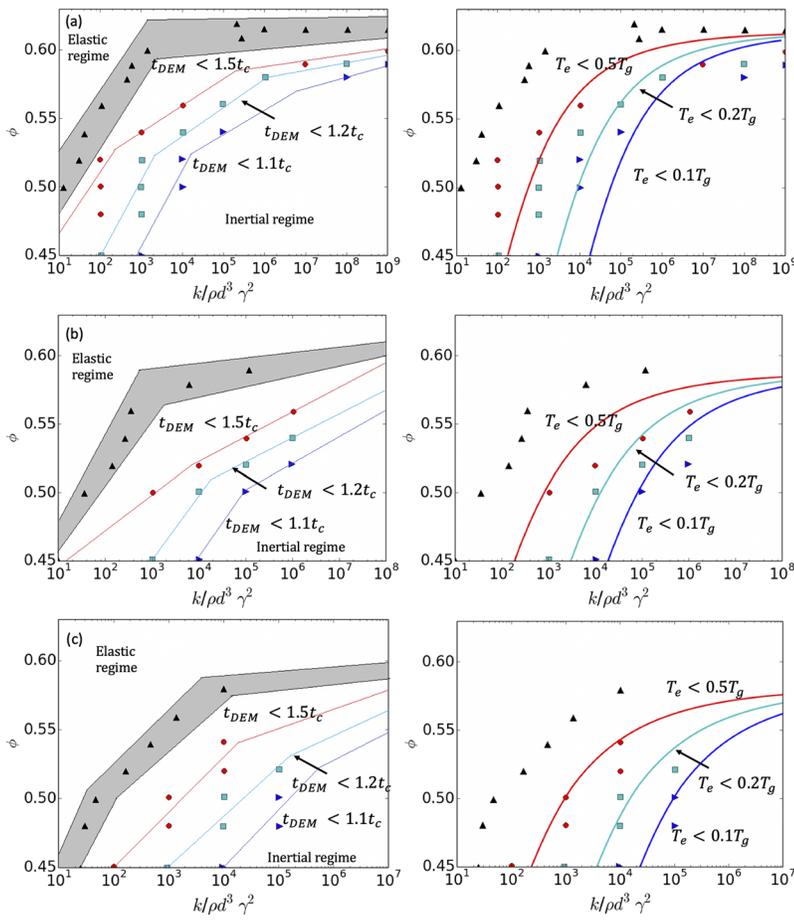


FIG. 6. Regime maps as presented by Campbell (Campbell 2002) based on DEM simulations (left column) and the presented model based on the ratio T_e/T_k (right column). $T_e/T_k = 0.1$: triangles; $T_e/T_k = 0.2$: squares; $T_e/T_k = 0.5$: circles. (a) $\mu = 0.1$, left: fit with DEM data from Campbell; right: drawing based on SSKT. (b) $\mu = 0.5$, left: fit with DEM data from Campbell; right: drawing based on SSKT. (c) $\mu = 1.0$, left: fit with DEM data from Campbell; right: drawing based on SSKT.

energy could be used to determine the granular flow regime. Here we use the ratio T_e/T_k from Eq. (20) as the parameter to determine the significance of the elastic effect in the inertial regime. For frictional granular systems, we use the modification proposed by Chialvo and Sundaresan,²¹ which includes the modified radial distribution function $g_{0,\mu}$ and energy balance equation between the granular temperature and shear rate,

$$g_{0,\mu} = \frac{1 - \frac{1}{2}\phi}{(1 - \phi)^3} + \frac{0.58\phi^2}{[\phi_c(\mu) - \phi]^{3/2}}, \quad (26)$$

where $\phi_c(\mu)$ is the μ dependent critical solid volume fraction.²¹

Based on the DEM simulation results, Campbell¹⁴ calculated the ratio of averaged contact time from DEM to the theoretical binary collision duration determined by the particle properties, t_{DEM}/t_c , to determine if the particle interactions are collisional. If all the collisions are binary, the actual contact time t_{DEM} must be equal to the binary collision duration, t_c . However, if the particles are involved in force chains in which particles endure longer contact time, one would expect the ratio $t_{DEM}/t_c > 1$. In theory, the KT model is only valid for collisional flows that correspond to $t_{DEM}/t_c = 1$; any value

larger than unity indicates non-binary collisional behavior, and the bulk behavior would be affected by not only the granular temperature but also the elastic properties of particles. In his work, three lines were added to the regime map, roughly pointing to the places where t_{DEM}/t_c falls below 1.5, 1.25, and 1.1, respectively. As the ratio becomes larger, the flow shows more elastic characteristics. A significant departure from the rapid flow behavior is observed when $t_{DEM}/t_c = 2$ at a solid fraction of 0.57.⁴³ Unlike their work in which the regime maps were drawn based on the DEM simulation results, here we quantitatively determine the extent of the elastic effect at the transition from inertial flows to elastic flows on the map based on the ratio T_e/T_k . Since T_e/T_k is proportional to the fraction of multi-body collisions as discussed in Sec. II, we expect the elastic granular temperature to be an alternative parameter that measures the elastic effect. As shown in the right column of Fig. 6, a very similar profile was observed as we change T_e/T_k from 0.1 to 0.5. This indicates that both T_e/T_k and t_{DEM}/t_c can be used to measure the extent of elastic effect in the system.

We also quantitatively compared our SSKT predictions with the DEM simulation results reported by Vescovi and

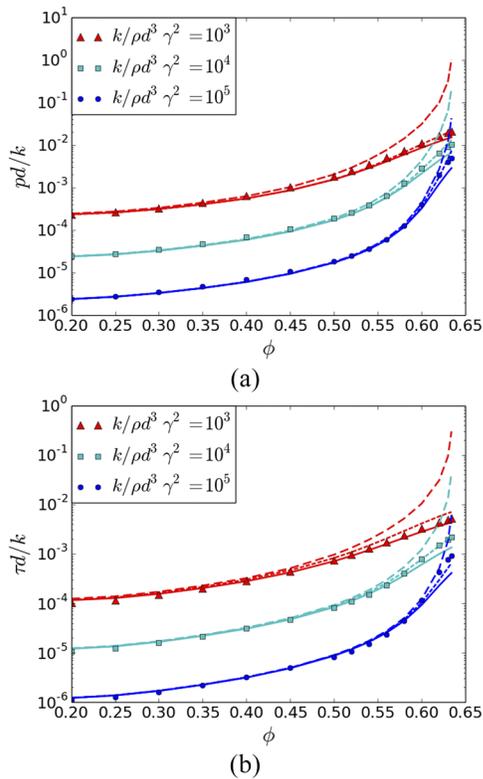


FIG. 7. Comparison between theoretical predictions and results from DEM simple shear simulations. Dots represent DEM data from Vescovi and Luding.⁴¹ Solid lines represent the SSKT prediction. Short dashed lines and long dashed lines represent the model by Berzi and Jenkins²³ and the classical KT, respectively. (a) Scaled pressure vs. solid volume fraction ϕ . (b) Scaled shear stress vs. solid volume fraction ϕ .

Luding⁴¹ In their work, simulations under uniform shear were conducted for frictionless spheres with $k/\rho d^3 \gamma^2$ ranging from 10^3 to 10^7 . We choose the cases with $k/\rho d^3 \gamma^2 = 10^3 - 10^5$ so that a large amount of elastic potential energy exists. The measured kinetic granular temperature is then used as an input to calculate the pressure and the shear stress. As shown in Fig. 7, for flows at a small solid volume fraction, t_c/t_f is negligible because the collision interval t_f is large and the results from both the KT model and the SSKT model could match the DEM results well. However, as ϕ becomes large, t_f will decrease and eventually become comparable to t_c ; in this case, the classical KT model over-predicts both pressure and shear stress and the discrepancy between the KT predictions and the DEM results becomes significant. It is also noticed that smaller k results in larger t_c/t_f and further increases the discrepancy. On the other hand, our SSKT model could predict the pressure and shear stress very well compared with the DEM simulation results. We conclude that the inclusion of particle stiffness into the KT model is very important for modeling granular flows away from the inertial limit; the SSKT model is able to capture the reduced pressure

and shear stress after considering the particle stiffness. The results from Berzi and Jenkins²³ model are also plotted in Fig. 7. For steady flows, the elastic granular temperature remains unchanged; both models modify solid stresses through the reduced collision frequency. Even though a new expression of the soft-particle collision frequency is used in the SSKT model, there is not much difference observed in the predicted pressures and stresses between the SSKT model and the Berzi and Jenkins model. However, it should be pointed out that a fitting contact duration $t_c = \frac{d}{5} \left(\frac{\rho \pi d}{4k} \right)^{\frac{1}{2}}$ is used in the Berzi and Jenkins model in order to match the DEM simulation results. This is not needed in our SSKT model since an accurate $t_c = \pi \left(\frac{k_n}{m_{\text{eff}}} - \frac{\eta_n}{4m_{\text{eff}}^2} \right)^{-\frac{1}{2}}$ for the LSD collision scheme has been used, which is consistent with t_c in DEM simulations. Compared with the Berzi and Jenkins model, the SSKT model can also predict the transfer between kinetic and elastic energy, which is very important for transient flows that have varying T_e . The comparison between two models for unsteady cooling cases will be discussed in Sec. III B.

B. Homogeneous cooling cases

For transient flows such as homogeneous cooling cases, T_e changes along with time, which means part of the elastic potential energy is being converted to the kinetic fluctuation energy during the cooling process. The change in T_k is a result of both inelastic collisions and energy transfer from T_e . The collision frequency is related to both the solid volume fraction and the kinetic granular temperature; it increases as the solid volume fraction or kinetic granular temperature increases, which means that the KT model can fail not only in the dense regime but also in the dilute regime at high granular temperature. The applicability of the KT model on uniform shear flows has been widely studied, but few studies have focused on the homogeneous cooling cases. As there is no driving force in a free cooling system, the initial granular temperature in the system will decrease due to inelastic collisions. Here we set up a three-dimensional free cooling system of fine particles. The system is dilute with a solid volume fraction $\phi = 0.2$ and particle restitution coefficient $e = 0.99$. We choose $e = 0.99$ so that the high granular temperature will dissipate slowly and the effect of the high collision frequency on soft-sphere systems can be more significant. The external force fields are ignored, and only the particle energy dissipation is considered. The DEM results are compared with the theoretical predictions of the SSKT model to investigate its accuracy in terms of predicting the energy dissipation rate. The change in total granular temperature T_g is equal to the energy dissipation rate of the system Γ . From Eq. (3), we have

$$\frac{d}{dt} \left[\frac{3}{2} \rho \phi \left(T_k + \frac{1}{3} T_e \right) \right] = -\Gamma, \quad (27)$$

and from the SSKT model, we have

$$T_e = KHT_k^{3/2}. \quad (28)$$

Combining Eqs. (27) and (28), the equation to solve T_k becomes

$$\frac{3}{2} \frac{dT_k}{dt} = \frac{12}{d\sqrt{\pi}} \phi g_0 (1 - e^2) \frac{T_k^{3/2}}{\left(1 + \frac{1}{2} KHT_k^{1/2}\right) \left[1 + (1 - \phi)KT_k^{1/2}\right]}, \quad (29)$$

where $g_0(\phi) = \frac{1 - \frac{1}{2}\phi}{(1 - \phi)^3}$ is the radial distribution function for cases with $\phi < 0.49$.⁴⁴

We first run the DEM simulation with low initial granular temperature $T_{k0} = 2 \times 10^{-4} \text{ m}^2/\text{s}^2$ and vary particle stiffness k from 10^2 N/m to 10^4 N/m . This also changes the binary collision duration t_c . As shown in Fig. 8(a), the KT predictions match the DEM results well when the initial granular temperature is relatively low such that the initial t_c/t_f is less than 0.05. During the cooling process, t_c/t_f is further decreased due to the decay of T_k , making t_c negligible. Contrary to the conventional wisdom, we find that the classical KT model can fail at low solid volume fractions if the particle collision frequency is sufficiently high (initial $t_c/t_f > 0.1$), as shown in Fig. 8(b), in which the initial granular temperature $T_{k0} = 2 \times 10^{-2} \text{ m}^2/\text{s}^2$.

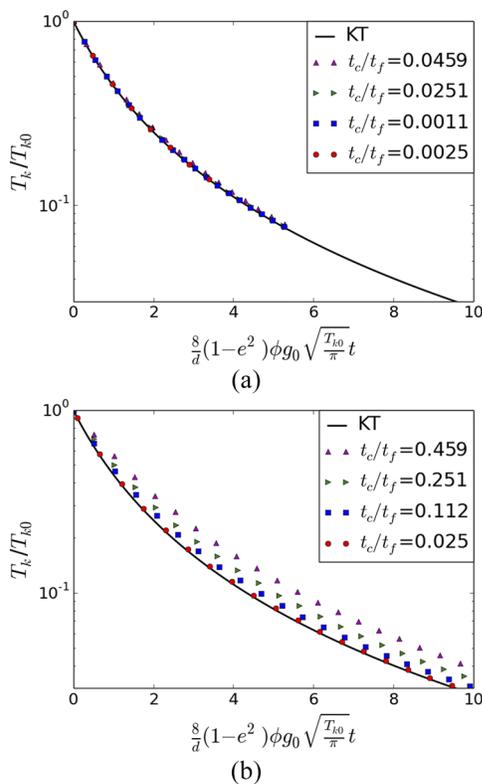


FIG. 8. Kinetic granular temperature T_k/T_{k0} as a function of rescaled time: $8/d(1 - e^2)\phi g_0 \sqrt{T_{k0}/\pi} t$ when the system is dilute and particles are nearly elastic ($\phi = 0.2$, $e = 0.99$). The solid line shows the prediction of the classical KT, and markers represent the DEM results. (a) $t_c/t_f < 0.05$ at low initial granular temperature $T_{k0} = 2 \times 10^{-4} \text{ m}^2/\text{s}^2$, different k has almost no impact on the results. (b) $t_c/t_f > 0.1$ at high initial granular temperature $T_{k0} = 2 \times 10^{-2} \text{ m}^2/\text{s}^2$, different k has a significant impact on the results if T_{k0} is large.

The KT prediction deteriorates because the increase in the collision frequency causes the collision interval to decrease, making the collision duration a parameter that can no longer be neglected when compared to the collision interval. Therefore, a large t_c/t_f at the initial stage increases the discrepancy between the predictions of the classical KT model and the DEM simulation results. As t_c/t_f increases due to the decrease in particle stiffness k , particles become softer and a significant amount of kinetic energy is converted into non-dissipative elastic energy, resulting in a larger portion of elastic potential energy or a larger T_e/T_k and a lower energy dissipation rate. At the same time, the collision frequency decreases, as shown in Eq. (23), and the energy dissipation rate is further reduced. From Fig. 9(a), we could see the classical KT can only match the result when t_c/t_f is very small. On the other hand, the SSKT model is able to include the effect of particle stiffness and provide better predictions even at large t_c/t_f . In Fig. 9(b), we also plot the results of the Berzi and Jenkins²³ model for the case of $t_c/t_f = 0.46$. Realizing that the velocity correlation

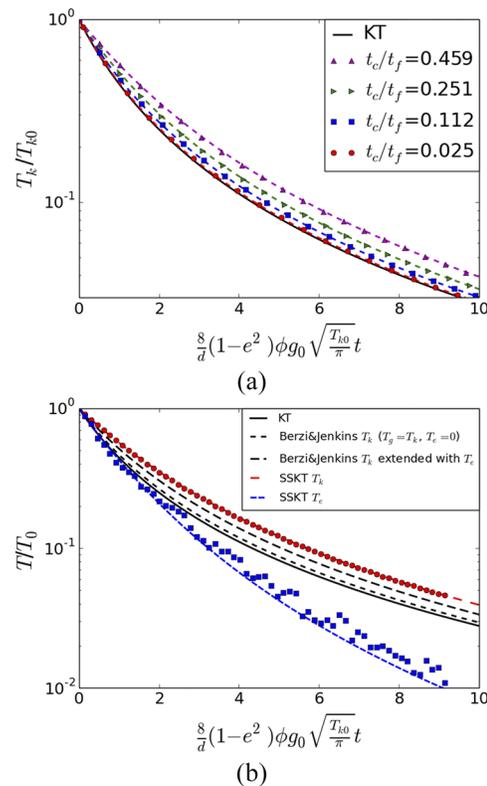


FIG. 9. Comparison between theoretical predictions and DEM results for homogeneous cooling cases. (a) Kinetic granular temperature T_k/T_{k0} as a function of rescaled time: $8/d(1 - e^2)\phi g_0 \sqrt{T_{k0}/\pi} t$ when the system is dilute and particles are nearly elastic. The solid line is the prediction of the classical KT, and dashed lines are results of the proposed SSKT model with different particle stiffness as the input. Markers represent the DEM simulation data. (b) T_k and T_e predicted by SSKT compared with DEM results (circles: T_k ; squares: T_e) and other models. $t_c/t_f = 0.459$.

should have no impact on flows without shear, we conclude that the energy dissipation rate of the homogeneous cooling flow is affected by the combination of the reduced collision frequency and existence of non-dissipative elastic energy. Since the Berzi and Jenkins model does not consider the effect of elastic potential energy, its prediction does not agree with the DEM simulations results. We extended Berzi and Jenkins model by considering $T_g = T_k + T_e/3$ and using the collision frequency expression in their model. During the cooling process, a large amount of elastic potential energy is converted to kinetic fluctuation energy. By including T_e into the granular temperature T_g , it can significantly decrease the discrepancy between the DEM and the theoretical prediction. However, there is still a difference between the predictions of the theory and the DEM because the reduced collision frequency is not accurately accounted for. On the other hand, by considering $T_g = T_k + T_e/3$ and using the proposed expression of the collision frequency from Eq. (23), the SSKT model is able to correctly predict the change in kinetic granular temperature as well as the elastic granular temperature during the cooling process.

IV. CONCLUSION

Finite particle stiffness makes sustained contacts possible. As a result, granular materials even in the dilute regime can exhibit both collisional and non-collisional behaviors. Flow regimes have commonly been used to better understand the hydrodynamic behaviors of different kinds of granular flows. For flows in the inertial regime, collisions can be treated as instantaneous events and the particle stiffness k would have less impact on the results, so the classical KT model can accurately capture the flow behavior and compare well with the DEM simulations. However, as flows move away from the inertial regime to the transition regime, the particle stiffness becomes critical in predicting the characteristics of granular flows. In some cases, the collision interval predicted by the KT model can be comparable to or even smaller than the collision time, which can be interpreted as the existence of enduring contacts between particles. Therefore, the modeling of granular flows in the transition regime has to consider the elastic properties of particles. In the present work, we have developed a SSKT model that takes the particle stiffness as an input parameter. The SSKT model extends the classical KT model by considering part of the kinetic fluctuation energy that actually exists in the form of elastic potential energy. This form of energy cannot be dissipated by collisions but can be transferred to the kinetic fluctuation energy spontaneously, which eventually affects the bulk behavior of granular flows. An elastic granular temperature is proposed to quantify the elastic potential energy in the system, and a correlation between the kinetic granular temperature and elastic granular temperature is derived based on the LSD collision scheme. In addition, an expression for the reduced collision frequency is proposed based on the DEM simulation results, which could be used to modify the pressure and stress in the SSKT model and to explain the change in granular flow behavior in the transition regime. We have shown that the SSKT model is able to

produce results that are in very good agreement with the DEM simulations. Considering the fact that granular flows of practical interest such as fluidized beds are unsteady and away from the inertial regime limit, the inclusion of particle stiffness into the continuum model allows us to improve the KT framework for a wider range of granular flows.

ACKNOWLEDGMENTS

This research work was supported by the U.S. Department of Energy.

APPENDIX: PARTICLE COLLISION FREQUENCY FROM KINETIC THEORY

For three-dimensional systems, the unperturbed particle distribution function could be written as

$$f(\mathbf{c}, \mathbf{r}, t) = n \left(\frac{1}{2\pi T_k} \right)^{3/2} \exp \left(- \frac{\mathbf{c}^2}{2T_k} \right), \quad (\text{A1})$$

where n is the particle number density and \mathbf{r} and \mathbf{c} are the position and velocity of each individual particle, respectively.

The collisional integration for the collision frequency is similar to the derivation of energy dissipation term, which can be found in the Appendix of another paper.³⁰ The total number of collisions per second in the system takes the form

$$\begin{aligned} \frac{dN_{\text{col}}}{dt} &= \frac{d^2}{2} \int d\mathbf{c}_1 \int d\mathbf{c}_2 \int_{\mathbf{c}_{12} \cdot \mathbf{k} < 0} (\mathbf{c}_{12} \cdot \mathbf{k}) g_0 n^2 \left(\frac{1}{2\pi T_k} \right)^3 \\ &\times \exp \left(- \frac{\mathbf{c}_1^2 + \mathbf{c}_2^2}{2T_k} \right) d\mathbf{k}. \end{aligned} \quad (\text{A2})$$

To obtain the integrations in Eq. (A2), we need to transform the integral variables $d\mathbf{c}_1 d\mathbf{c}_2$ to $d\mathbf{c}_{12} d\mathbf{c}'_{12}$, where $\mathbf{c}_1 = \frac{\mathbf{c}'_{12} + \mathbf{c}_{12}}{2}$ and $\mathbf{c}_2 = \frac{\mathbf{c}'_{12} - \mathbf{c}_{12}}{2}$. The Jacobian of this transformation is $1/8$. We obtain

$$\frac{dN_{\text{col}}}{dt} = 2\pi^{1/2} d^2 n^2 g_0 T_k^{1/2}. \quad (\text{A3})$$

The collision frequency is defined as the number of collisions per particle, so we need to divide the number of collisions by the particle number density n , and $n = \frac{6\phi}{\pi d^3}$. Finally, we have

$$f_{\text{KT}} = \frac{1}{n} \frac{dN_{\text{col}}}{dt} = \frac{12}{d} \phi g_0 \sqrt{\frac{T_k}{\pi}}. \quad (\text{A4})$$

REFERENCES

- ¹C. Lun, S. B. Savage, D. Jeffrey, and N. Chepurnyi, "Kinetic theories for granular flow: Inelastic particles in couette flow and slightly inelastic particles in a general flowfield," *J. Fluid Mech.* **140**, 223 (1984).
- ²J. T. Jenkins and S. B. Savage, "A theory for the rapid flow of identical, smooth, nearly elastic, spherical particles," *J. Fluid Mech.* **130**, 187 (1983).
- ³S. McNamara and W. Young, "Inelastic collapse in two dimensions," *Phys. Rev. E* **50**, R28 (1994).
- ⁴S. Luding and S. McNamara, "How to handle the inelastic collapse of a dissipative hard-sphere gas with the TC model," *Granular Matter* **1**, 113 (1998).

- ⁵P. A. Cundall and O. D. Strack, "A discrete numerical model for granular assemblies," *Geotechnique* **29**, 47 (1979).
- ⁶J. J. Moreau, "Unilateral contact and dry friction in finite freedom dynamics," in *Nonsmooth Mechanics and Applications* (Springer, 1988), pp. 1–82.
- ⁷M. Jean, "The non-smooth contact dynamics method," *Comput. Methods Appl. Mech. Eng.* **177**, 235 (1999).
- ⁸C. S. Campbell, "Rapid granular flows," *Annu. Rev. Fluid Mech.* **22**, 57 (1990).
- ⁹N. Mitarai and H. Nakanishi, "Hard-sphere limit of soft-sphere model for granular materials: Stiffness dependence of steady granular flow," *Phys. Rev. E* **67**, 021301 (2003).
- ¹⁰N. Mitarai and H. Nakanishi, "Bagnold scaling, density plateau, and kinetic theory analysis of dense granular flow," *Phys. Rev. Lett.* **94**, 128001 (2005).
- ¹¹L. E. Silbert, G. S. Grest, R. Brewster, and A. J. Levine, "Rheology and contact lifetimes in dense granular flows," *Phys. Rev. Lett.* **99**, 068002 (2007).
- ¹²N. Mitarai and H. Nakanishi, "Velocity correlations in dense granular shear flows: Effects on energy dissipation and normal stress," *Phys. Rev. E* **75**, 031305 (2007).
- ¹³P. Si, H. Shi, and X. Yu, "Development of a mathematical model for submarine granular flows," *Phys. Fluids* **30**, 083302 (2018).
- ¹⁴C. S. Campbell, "Granular shear flows at the elastic limit," *J. Fluid Mech.* **465**, 261 (2002).
- ¹⁵S. Chialvo, J. Sun, and S. Sundaresan, "Bridging the rheology of granular flows in three regimes," *Phys. Rev. E* **85**, 021305 (2012).
- ¹⁶F. Da Cruz, S. Emam, M. Prochnow, J.-N. Roux, and F. Chevoir, "Rheo-physics of dense granular materials: Discrete simulation of plane shear flows," *Phys. Rev. E* **72**, 021309 (2005).
- ¹⁷P. Jop, Y. Forterre, and O. Pouliquen, "A constitutive law for dense granular flows," *Nature* **441**, 727 (2006).
- ¹⁸N. Martin, I. Ionescu, A. Mangeney, F. Bouchut, and M. Farin, "Continuum viscoplastic simulation of a granular column collapse on large slopes: μ (I) rheology and lateral wall effects," *Phys. Fluids* **29**, 013301 (2017).
- ¹⁹S. Mandal and D. Khakhar, "A study of the rheology of planar granular flow of dumbbells using discrete element method simulations," *Phys. Fluids* **28**, 103301 (2016).
- ²⁰T. Barker, D. Schaeffer, P. Bohorquez, and J. Gray, "Well-posed and ill-posed behaviour of the $\mu(I)$ -rheology for granular flow," *J. Fluid Mech.* **779**, 794 (2015).
- ²¹S. Chialvo and S. Sundaresan, "A modified kinetic theory for frictional granular flows in dense and dilute regimes," *Phys. Fluids* **25**, 070603 (2013).
- ²²D. Vescovi, D. Berzi, P. Richard, and N. Brodu, "Plane shear flows of frictionless spheres: Kinetic theory and 3D soft-sphere discrete element method simulations," *Phys. Fluids* **26**, 053305 (2014).
- ²³D. Berzi and J. T. Jenkins, "Steady shearing flows of deformable, inelastic spheres," *Soft Matter* **11**, 4799 (2015).
- ²⁴L. Kondic and R. Behringer, "Elastic energy, fluctuations and temperature for granular materials," *Europhys. Lett.* **67**, 205 (2004).
- ²⁵H. H. Shen and B. Sankaran, "Internal length and time scales in a simple shear granular flow," *Phys. Rev. E* **70**, 051308 (2004).
- ²⁶Q. Sun, F. Jin, and G. G. Zhou, "Energy characteristics of simple shear granular flows," *Granular Matter* **15**, 119 (2013).
- ²⁷S. Benyahia, M. Syamlal, and T. O'Brien, "Summary of MFIx equations 2012-1," from <https://mfix.netl.doe.gov/documentation/MFIxEquations2012-1.pdf>, 2012.
- ²⁸M. Babic, "Average balance equations for granular materials," *Int. J. Eng. Sci.* **35**, 523 (1997).
- ²⁹R. Artoni and P. Richard, "Average balance equations, scale dependence, and energy cascade for granular materials," *Phys. Rev. E* **91**, 032202 (2015).
- ³⁰Y. Duan and Z.-G. Feng, "Incorporation of velocity-dependent restitution coefficient and particle surface friction into kinetic theory for modeling granular flow cooling," *Phys. Rev. E* **96**, 062907 (2017).
- ³¹S. Torquato, "Nearest-neighbor statistics for packings of hard spheres and disks," *Phys. Rev. E* **51**, 3170 (1995).
- ³²Y. Duan, Z.-G. Feng, E. E. Michaelides, and S. Mao, "Modified kinetic theory applied to the shear flows of granular materials," *Phys. Fluids* **29**, 043302 (2017).
- ³³M. Syamlal, W. Rogers, and T. J. O'Brien, "MFIx documentation: Theory guide national energy technology laboratory," Technical Note DOE/METC-95/1013 and NTIS/DE95000031, Department of Energy, 1993.
- ³⁴L. E. Silbert, D. Ertaş, G. S. Grest, T. C. Halsey, D. Levine, and S. J. Plimpton, "Granular flow down an inclined plane: Bagnold scaling and rheology," *Phys. Rev. E* **64**, 051302 (2001).
- ³⁵Y. Gu, A. Ozel, and S. Sundaresan, "A modified cohesion model for CFD-DEM simulations of fluidization," *Powder Technol.* **296**, 17 (2016).
- ³⁶V. Garzó and J. Dufty, "Dense fluid transport for inelastic hard spheres," *Phys. Rev. E* **59**, 5895 (1999).
- ³⁷J. T. Jenkins and D. Berzi, "Dense inclined flows of inelastic spheres: Tests of an extension of kinetic theory," *Granular Matter* **12**, 151 (2010).
- ³⁸J. T. Jenkins, "Dense shearing flows of inelastic disks," *Phys. Fluids* **18**, 103307 (2006).
- ³⁹J. T. Jenkins, "Dense inclined flows of inelastic spheres," *Granular Matter* **10**, 47 (2007).
- ⁴⁰D. Berzi, "Extended kinetic theory applied to dense, granular, simple shear flows," *Acta Mech.* **225**, 2191 (2014).
- ⁴¹D. Vescovi and S. Luding, "Merging fluid and solid granular behavior," *Soft Matter* **12**, 8616 (2016).
- ⁴²C. S. Campbell, "Granular material flows—an overview," *Powder Technol.* **162**, 208 (2006).
- ⁴³Y. Zhang and C. S. Campbell, "The interface between fluid-like and solid-like behaviour in two-dimensional granular flows," *J. Fluid Mech.* **237**, 541 (1992).
- ⁴⁴N. F. Carnahan and K. E. Starling, "Equation of state for nonattracting rigid spheres," *J. Chem. Phys.* **51**, 635 (1969).