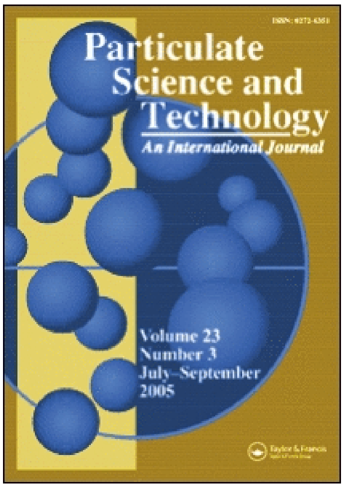

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Energy Conservation in a Granular Shear Flow and Its Quasi-Solid-Liquid Transition

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Energy conservation and the quasi-solid-liquid transition are studied for a nonuniform granular shear flow in nonequilibrium steady state using 3-D discrete element simulation. Energy fluctuation and its relation to interparticle force chains are discussed. Sensitivity analyses are carried out of energy to different parameters, such as concentration, restitution coefficient, and friction coefficient. Elastic potential energy distribution in the quasi-solid-liquid transition is discussed, and the inherent fundamental mechanisms of transition from the perspective of energy are developed.

Keywords discrete element method, energy conservation, granular materials, nonequilibrium steady state, quasi-solid-liquid transition

Introduction

Granular materials are of interest in a wide range of research fields, such as natural ecology, industry processes, and life science (Pouliquen et al. 2006). With various material properties and external driving forces, granular materials exhibit various mechanical behaviors at macroscale (Jameger & Nagel 1992). But at microscale, particle motions and their interactions obey a basic law, that is, energy conservation (Luding & Herrmann 1999; Peng & Ohta 1998). As a relatively complex energy dissipative system, the main energy dissipative paths are through interparticle nonelastic collisions and shear sliding frictions. When the external power input just balances the energy dissipation rate, the total internal energy (sum of the elastic potential energy and the kinetic energy) stabilizes gradually, and the granular system arrives at a nonequilibrium steady state. Therefore, the energy distribution and its conservation play an important role in the study of granular flow dynamics. It has been found that energy dissipation rate is closely

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related to material properties, shear rates, and concentrations of the granular system (Krouskop & Talbot 2004; Zhang & Rauenzahn 2000).

Granular materials behave like a solid or a liquid under different concentrations, shear rates, and constraints. Quasi-solid-liquid transition may occur under a certain kind of condition (Campbell 2002; Jop et al. 2006; Orpe & Khakhar 2004). Many numerical simulations and experimental verifications have been devoted to this transition of granular media. Usually, the flow has been characterized by the intensity of the force chain, contact time, and the space orientation in terms of macro-stress or effective friction coefficient (i.e., the ratio of shear stress to normal stress), contact time number, and coordination number (Babic et al. 1990; Campbell 2002, 2006; GDR MiDi 2004). As being a typical energy dissipative system, the quasi-solid-liquid transition of granular media will be investigated from the viewpoint of energy. This transition is also a nonequilibrium one since the energy dissipation accompanies the whole process of granular flow, which is irreversibly nonequilibrium. Some of the fundamental aspects related to energy propagation, fluctuation, and distribution have been reported earlier (Brey et al. 2004; Jalali et al. 2003; Peng & Ohta 1998). However, the inherent mechanism of the quasi-solid-liquid transition has not been explored through energy approach.

Therefore, the objective of this study is to gain an insight into energy conservation and the quasi-solid-liquid transition of granular flows from the perspective of energy. The energy dissipation rate and external power input are first calculated to verify energy conservation based on the simulations of a granular shear flow in steady state using the 3-D discrete element method. The relationship between energy fluctuations and force chains is discussed. Next, sensitivity analyses are performed of energy distribution to concentrations, friction coefficients, and restitution coefficients. Finally, energy distribution, in particular, elastic potential energy distribution, which is the intrinsic characteristic of the quasi-solid-liquid transition, is discussed.

Basic Equations of Granular Flow Dynamics

Since it was first established in 1970s by Peter Cundall, the discrete element method (DEM) has been used widely in such fields as rock engineering, powder materials, chemical processing, traffic flow, and earth science. In this study, 3-D DEM is adopted to simulate collisions and motions between particles. Energy conservation and quasi-solid-liquid transition are addressed based on the calculations of new introduced dimensionless variables.

Contact Force Model of Particle Collision

The contact force model is determined by material properties of particles and the physical contact process between particles. In actual application, a nonlinear model is more reasonable for interparticle collisions. But in the study of dynamics of granular materials, the linear viscous-elastic model is more convenient, because the restitution coefficient and contact time can be defined directly and the simulated results can reasonably represent macro-mechanical behaviors of granular materials (Ji & Shen 2006). Thus, the linear viscous-elastic contact force model based on Mohr-Coulomb friction law is widely adopted in granular flow dynamics (Babic et al. 1990; Campbell 2006; Ji & Shen 2006).

In the collision of two particles, the normal contact force consists of the normal elastic force and the normal viscous force (Babic et al. 1990):

$$F_n = F_n^e + F_n^v \tag{1}$$

where the normal elastic force $F_n^e = K_n x_n$ and the normal viscous force $F_n^v = C_n \dot{x}_n$. Here, x_n and $\dot{x}_n$ are the relative normal displacement and the relative normal velocity between particles, respectively. K_n and C_n are the normal stiffness and damping coefficient. The damping coefficient is given by Babic et al. (1990)

$$C_n = \zeta_n \sqrt{2MK_n} \tag{2}$$

$$\zeta_n = \frac{-\ln e}{\sqrt{\pi^2 + \ln^2 e}} \tag{3}$$

where ζ_n is the dimensionless damping coefficient, e is the coefficient of restitution, and M is the effective mass of the two particles.

Based on the Mohr-Coulomb friction law, the tangential force can be determined by Babic et al. (1990)

$$F_s = \begin{cases} F_s^* & \text{if } |F_s^*| \le \mu F_n^e \\ \text{sign}(F_s^*)\mu F_n^e & \text{if } |F_s^*| > \mu F_n^e \end{cases} \tag{4}$$

where $F_s^* = K_s x_s$. Here, x_s is the relative tangential displacement between particles, K_s is the tangential stiffness and $K_s = \alpha K_n$, α is chosen to be 0.8 (Babic et al. 1990; Campbell 2002), and μ is the friction coefficient.

Energy Equations of Dynamics of Granular Shear Flow

In the dynamics of granular flows, total energy includes elastic potential energy and kinetic energy. The viscous collision and the sliding friction are the two contributors of energy dissipation. For a granular shear flow, the external energy input (or work done by the external force) is supplied by the shear stress. Thus, the energy equation can be written as Babic et al. (1990)

$$\frac{\mathrm{d}(T + P)}{\mathrm{d}t} = W - \Gamma \tag{5}$$

where T is the kinetic energy per unit volume, P is the potential energy per unit volume, W is the power input by external driving forces per unit volume, and Γ is the energy dissipation rate per unit volume. The total energy is the sum of kinetic energy and potential energy, that is, $E = T + P$.

In the present 3-D granular system with period boundaries subject to shearing, the power input by the external force can be written as Babic et al. (1990)

$$W = \sigma_{ji} S_{ij} \tag{6}$$

where σ_{ji} is the macro-stress tensor and s_{ji} is the strain rate tensor. The matrix of strain rate tensor is

$$S_{ij} = \begin{bmatrix} 0 & \dot{\gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{7}$$

where $\dot{\gamma}$ is the shear rate of the granular system.

The macro-stress of the granular system consists of two terms: contact stress and kinetic stress. That is (Babic et al. 1990; Campbell 2006),

$$\sigma_{ij} = \sigma_{ij}^c + \sigma_{ij}^k \tag{8}$$

where σ_{ij}^c and σ_{ij}^k are the contact stress tensor and the kinetic stress tensor, respectively. These terms are given by

$$\sigma_{ij}^c = \frac{1}{V}\sum_{k=1}^{N}\sum_{l=1}^{N_k}(r_i^{lk}F_j^{kl}) \tag{9}$$

$$\sigma_{ij}^k = \frac{1}{V}\sum_{k=1}^{N}M_k(u_i'^k u_j'^k) \tag{10}$$

where V is the volume of computation domain, N is the particle number, N_k is the contact number with particle k, M_k is the mass of particle k, r_i^{lk} is the position tensor from the center of particle l to the center of particle k, F_j^{kl} is the tensor of the total force exerted by particle l on particle k, and $u_i'^k$ and $u_j'^k$ are the fluctuating velocity tensors of particle k.

The kinetic energy, potential energy, and energy dissipation rate per unit volume are expressed as follows (Babic et al. 1990):

$$T = \frac{1}{V}\sum_{p=1}^{N}\frac{1}{2}(M_p\dot{u}_p^2 + I_p\dot{\theta}_p^2) \tag{11}$$

$$P = \frac{1}{V}\left[\sum_{c=1}^{N_c}\frac{1}{2}(K_n x_n^2) + \sum_{c=1}^{N_{c1}}\frac{1}{2}(K_s x_s^2)\right] \tag{12}$$

$$\Gamma = \frac{1}{V}\left[\sum_{c=1}^{N_c}\frac{1}{2}(C_n\dot{x}_n^2) + \sum_{c=1}^{N_{c2}}\frac{1}{2}(\mu K_n x_n|\dot{x}_s|)\right] \tag{13}$$

where u_p and $\dot{\theta}_p$ are the translational and angular velocities of particle p, I_p is the moment of inertia of particle p, N_c is the total number of contacts within the computation domain, N_{c1} is the number of non-sliding contacts, and N_{c2} is the number of sliding contacts. It can be seen from Equations (11)–(13) that the kinetic energy of the granular system T includes the translational kinetic energy T_t and the rotational kinetic energy T_r. The elastic potential energy P includes the normal elastic energy P_n and the tangential elastic energy P_s. The energy dissipation rate Γ includes the energy dissipated by the inelastic collision Γ_c and by the sliding friction Γ_f.

Energy Conservation in Granular Shear Flow and Sensitivity Analysis

Granular shear flow with periodic boundary conditions is simulated with 3-D DEM in order to study energy conservation of a granular system in nonequilibrium steady state. The potential energy, kinetic energy, energy dissipation rate, and power input by the external force are calculated, and the effects of different material properties on energy distributions are discussed.

Granular Steady-State Flow Process and Its Energy Conservation

In the computation domain of $a \times b \times c = 10\widetilde{D} \times 10\widetilde{D} \times 10\widetilde{D}$ of the granular system with periodic boundary conditions, nonuniform particles are placed randomly under different concentrations. Here, $\widetilde{D}$ is the mean particle diameter and has a uniform probability distribution in the range of $[0.9\widetilde{D}, 1.1\widetilde{D}]$. The granular system is sheared with a shear rate of $\dot{\gamma} = V/b$ in y direction. V is the relative velocity of the upper and lower boundaries. The main parameters used in the simulation are listed in Table 1.

In order to fully analyze the effect of every parameter on the energy process of the granular system in steady state, new dimensionless variables are introduced. They are dimensionless stress $\sigma^*_{ij} = \sigma_{ij}/\rho\widetilde{D}^2\dot{\gamma}^2$, dimensionless stiffness $K^*_n = \widetilde{K}_n/\rho\widetilde{D}^3\dot{\gamma}^2$, dimensionless energy dissipation rate per unit volume $\Gamma^* = \Gamma/\rho\widetilde{D}^2\dot{\gamma}^3$, dimensionless potential energy per unit volume $P^* = P/\rho\widetilde{D}^2\dot{\gamma}^2$, and dimensionless kinetic energy per unit volume $T^* = T/\rho\widetilde{D}^2\dot{\gamma}^2$. Similarly, dimensionless energy components of Γ^*_C and Γ^*_f, T^*_t and T^*_r, P^*_n and P^*_s and dimensionless stress components σ^{*C}_{ij} and σ^{*K}_{ij} can be obtained. In the shear process, the nominal strain is taken as $\gamma = \dot{\gamma}t$, where t is the computation time. Here, the nominal strain can be treated as a dimensionless strain and used to analyze dynamic process of the above dimensionless variables (Campbell 2002; Jalali et al. 2003).

Dimensionless energy dissipation rate Γ^* and external power input W^*, potential energy P^*, kinetic energy T^*, and total energy E^* are first calculated and plotted in Figure 1(a) and (b). It is shown that energy dissipation rate and external power input are in dynamic equilibrium and have similar average values. So energy is conserved and the granular system exhibits a steady-state flow.

Components of these dimensionless variables (Γ^*_C and Γ^*_f, T^*_t and T^*_r, P^*_n and P^*_S, σ^{*c}_{ij} and σ^{*K}_{ij}) are given in Figures 1(c)–(h). It is observed that these components all maintain their own stable fluctuations, which guarantees the steady state of the whole granular system. Moreover, from the magnitude of each component, it can be seen that energy dissipation rate caused by friction, translational energy, normal elastic potential energy, and contact stress are apparently larger than the energy dissipation rate caused by inelastic collision, rotational energy, tangential elastic potential energy, and kinetic stress, respectively. These are key factors that influence the flow state of a granular system.

In addition, it can be seen from Figure 1 that all the above variables exhibit fluctuations around their average values. This fluctuation phenomenon exists widely

Table 1. Main parameters used in DEM simulation

Variable	Definition	Value
$\widetilde{D}$	Mean particle diameter	0.01 m
$a \times b \times c$	Computation domain	$0.1 \times 0.1 \times 0.1$ m
$\widetilde{K}_n$	Mean stiffness coefficient	1.0×10^4 N/m
ρ	Density	1.0×10^3 kg/m^3
μ	Friction coefficient	0.5
e	Restitution coefficient	0.7
$\dot{\gamma}$	Shear rate	31.62 s^{-1}
C	Concentration	0.60

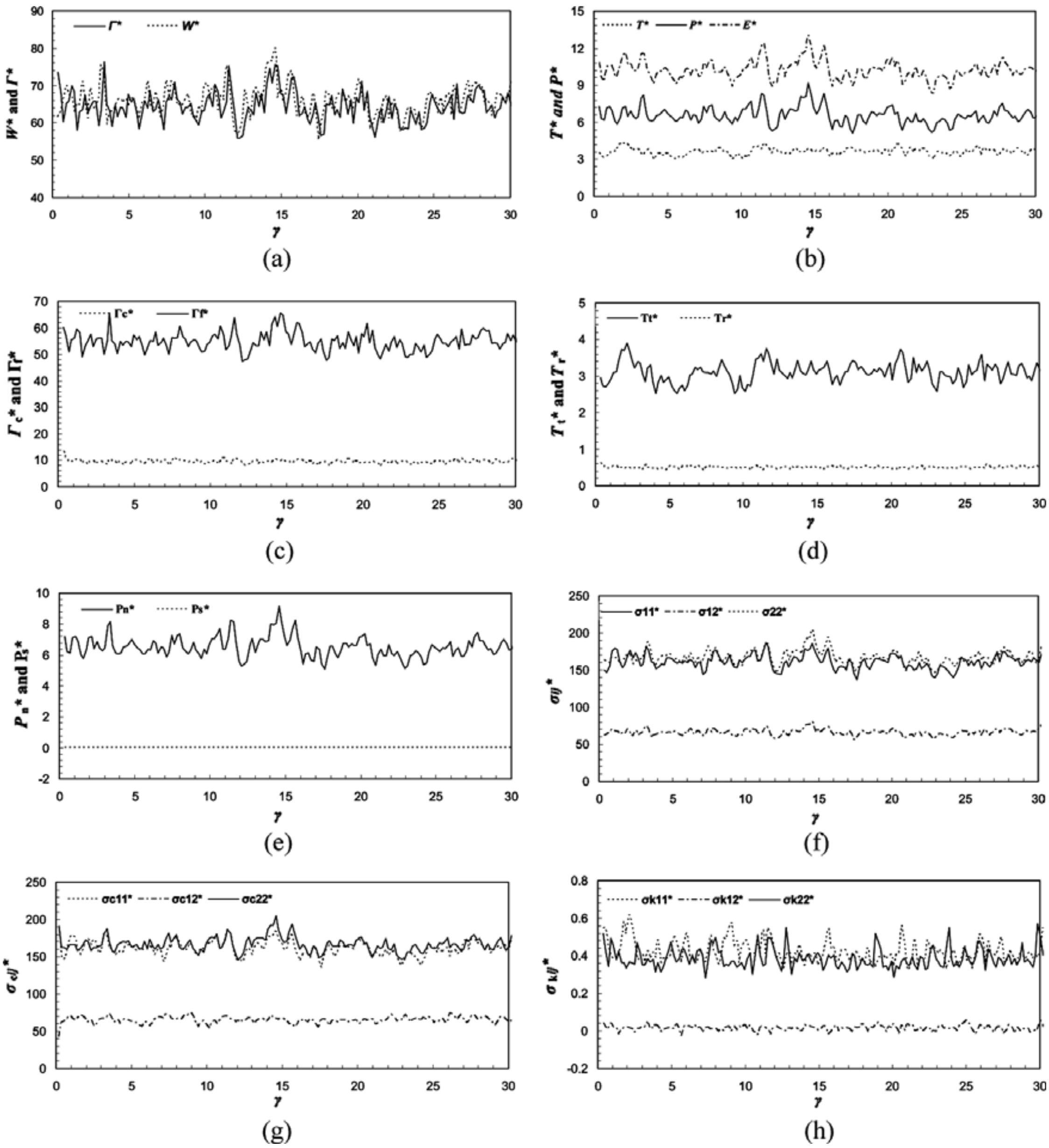

Figure 1. Energy dissipation rate, external power input, kinetic energy, potential energy, total energy, macro-stress, and their components in the dynamic equilibrium of a simple shear granular system.

in dynamics of granular systems, and the fluctuation amplitude usually increases with the increase of concentration (Jalali et al. 2003).

Fluctuations of particle velocity, force chain intensity, and macro-stress and their probability distributions have been studied thoroughly at different scales (Dalton et al. 2005; Howell et al. 1999; Rouyer & Menon 2000). It is well known that fluctuations in granular media at macroscale are closely related to contacts of particles at microscale, that is, force chain intensity, concentration, and space orientation (Goldenberg & Goldhirsch 2002; Luding 2005). Therefore, the formation, persistence, and splitting of force chains and their orientation determine the way of the internal force transmission and further influence the macro-flow of granular media.

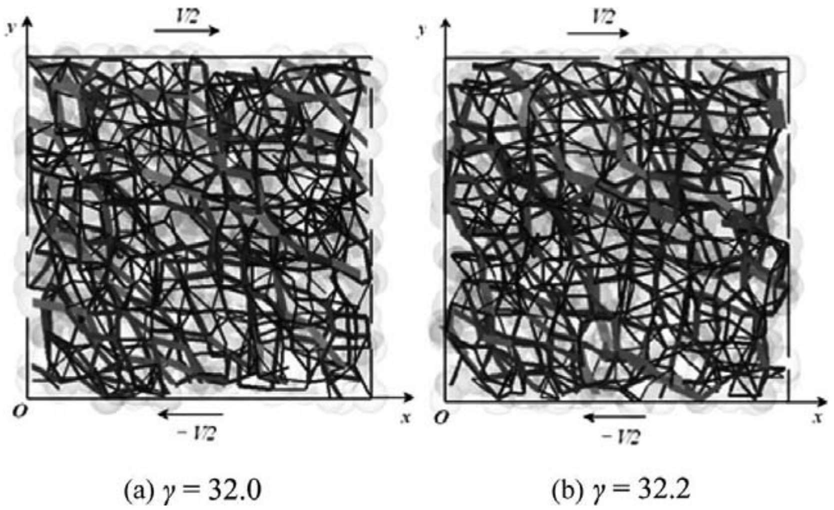

Figure 2. Sketch of the normal contact force chain of granular shear flow in steady state.

In order to better understand fluctuations in granular media, two instantaneous force chains (nominal strain) are shown in Figures 2(a) and (b). It can be seen that force chains show remarkable anisotropy spatially at microscale and mainly carry the shear force induced by the relative movements of particles at different layers. Taking a closer look at Figure 2(a) and (b), it can be observed that principal force chains exhibit strong similarity spatially, but the concrete arrangement and intensity distribution are very different. It is the spatial and temporal random distributions that generate certain fluctuations in granular media.

Fluctuations of granular media occur near their equilibrium point, and this equilibrium location is the characteristic of granular flow in steady state. Although the flow state may show great differences with different material properties, the energy dissipation and work done by external forces obey the law of energy conversation for granular systems in any steady state. This guarantees the relative stability of the system.

Parameter Sensitivity Analysis of Energy Conservation

With different particle properties (such as stiffness coefficient, restitution coefficient, friction coefficient, particle size, and density) and flow states (such as shear rate and concentration), the intensity, frequency, and duration of interparticle collisions and the cluster structure vary accordingly, which will change the distribution of the stored potential energy, energy dissipation rate, and work done by external forces. This section focuses on the effects of different parameters on energy distributions.

A reference shear granular system of $C = 0.60$, $K_n^* = 1.0 \times 10^4$, $\mu = 0.50$, and $e = 0.70$ is first established. Based on this reference system, different values of concentration C ($C = 0.40, 0.50, 0.60, 0.65$), dimensionless stiffness K_n^* ($K_n^* = 1.0 \times 10^2, 1.0 \times 10^4, 1.0 \times 10^6$), restitution coefficient e ($e = 0.1, 1.0$), and friction coefficient μ ($\mu = 0.1, 0.5, 0.75$) are selected to perform parameter sensitivity analysis of energy distributions. Figure 3 shows the distribution of the energy dissipation rate Γ^*, external power input W^*, total energy E^*, and macro-stress σ_{22}^* with the effects of the selected parameters. It can be found the energy dissipation

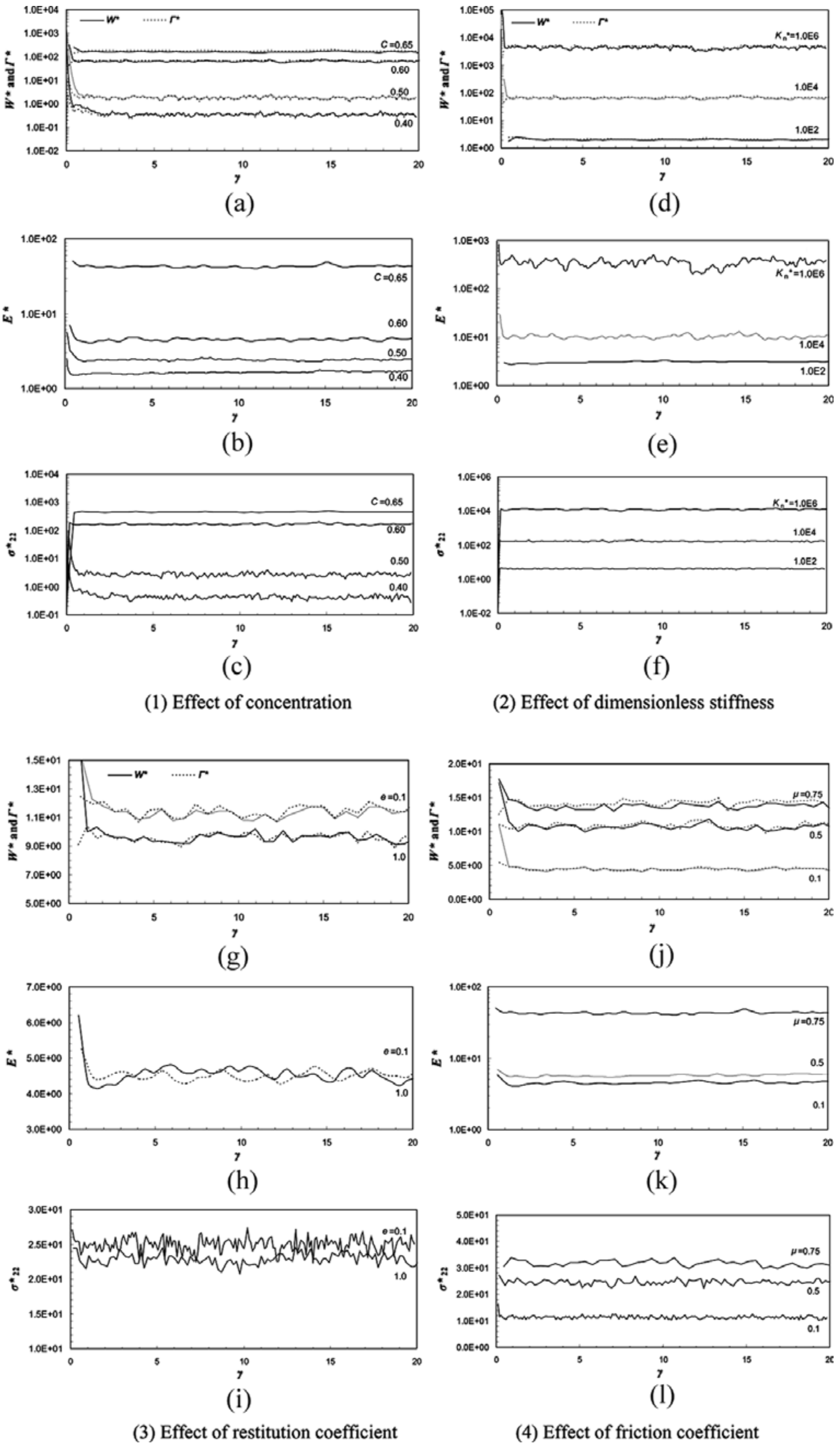

Figure 3. Energy dissipation rate, external power input, total energy, and macro-stress simulated with different parameters.

rate equals the power input, that is, energy is conserved in the steady state of granular shear flow.

It can also be seen from Figure 3 that dimensionless energy dissipation rate Γ^*, external power input W^*, total energy E^*, and macro-stress σ_{22}^*, on one hand, increase with the increase of concentration C, dimensionless stiffness K_n^*, and friction coefficient μ; on the other hand, they increase with the decrease of restitution coefficient e. This suggests that:

1. At the same shear rate, with the increase of concentration, the frequency, contact duration, and amplitude of interparticle collisions increase accordingly and induce the increase of total internal energy E^*, energy dissipation rate Γ^*, and macro-stress σ_{22}^*.
2. At the same shear rate and concentration, the contact force increases with the increase of mean stiffness coefficient $\widetilde{K}_n$. The elastic potential energy, macro-stress, energy dissipation rate, and external power input will also increase. In fact, at different shear rates and concentrations, $\widetilde{K}_n$ has a different influence on energy components due to the different flow phases. This can be fully demonstrated in the next section of the quasi-solid-liquid transition study of granular media.
3. When friction coefficient increases, shear force increases obviously and causes elastic tangential potential energy and sliding friction energy to increase. The total energy and macro-stress of the system will also increase. In granular flow dynamics, the friction coefficient is one of the most important factors that influence mechanical behaviors of granular media (Goldenberg & Goldhirsch 2005).
4. The decrease of restitution coefficient produces more persistent contacts and increases energy dissipation rate and external driving power needed due to the increase of viscous force. Meanwhile, kinetic energy has obvious tendency of decrease and causes the decrease of the total energy of the granular system.

Energy Distribution in Quasi-Solid-Liquid Transition

Mechanical behavior of dry, cohesionless granular material can be classified into rapid, slow, and quasi-static regimes (Babic et al. 1990). The quasi-solid-liquid transition is one of the unique properties of granular media and is widely investigated in different research areas (Babic et al. 1990; Campbell 2006; Hou et al. 2003). This transition was usually studied through the intensity, contact time, and spatial structure of force chains by means of macro-stress, contact time number, and coordination number (Babic et al. 1990; Campbell 2002, 2006). Actually, as a complex energy dissipative system, energy dissipation and external energy input accompanies the whole flow process of the granular system, including the quasi-solid-liquid transition. Clearly, this transition is a typical nonequilibrium one, and the flow state is closely related to the energy distribution of the granular system. Therefore, it would be very helpful to investigate the quasi-solid-liquid transition from the viewpoint of energy in order to better understand the intrinsic characteristics of phase transition.

Using the nonuniform granular shear flow model established above, dimensionless macro-stress components σ_{12}^* and σ_{22}^* are simulated and plotted in Figure 4(a) and (b) versus dimensionless stiffness K_n^* with different concentrations. It can be observed that at low concentration ($C = 0.40$), σ_{12}^* and σ_{22}^* are independent

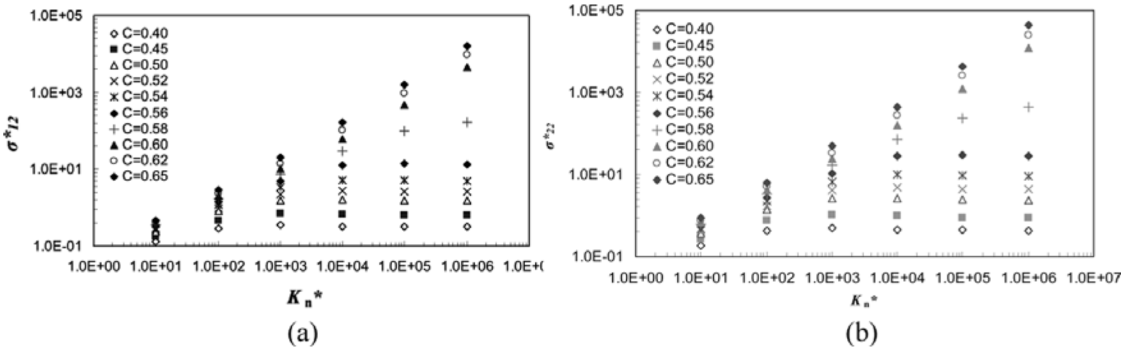

Figure 4. Plots of dimensionless macro-stress vs. dimensionless stiffness with different concentrations.

of K_n^* and proportional to the square of shear rate. Under this condition, the granular system exhibits rapid flow and behaves like a liquid. At high concentration ($C = 0.65$), the $\sigma_{ij}^* - K_n^*$ plot indicates a log-linear relationship, the slope of which is found to be 1. The granular system presents quasi-static flow and behaves like a solid. At medium concentration, σ_{ij}^* is independent of K_n^* with higher K_n^* and the $\sigma_{ij}^* - K_n^*$ plot is a log-linear one with lower K_n^*. Therefore, when K_n^* changes from low to high, that is, shear rates change from high to low, quasi-solid-liquid transition may occur.

Macro-stress is the extrinsic characteristic in the quasi-solid-liquid transition of granular media. The intrinsic factor should be the different distribution of elastic potential energy induced by particle collision frequencies, intensity of force chains, and space orientations at different concentrations and shear rates. Therefore, elastic potential energy would fully reflect the quasi-solid-liquid transition of the granular system. The simulated elastic potential energy P^* and its components P_n^* and P_s^* are given in Figure 5.

It can be seen in Figure 5 that potential energy components P_n^* and P_s^* both have the same distribution as total potential energy P^*. Figures 5(a), (c), and (e) show that at high concentration ($C = 0.65$), dimensionless potential energy P^* increases with the increase of dimensionless stiffness K_n^* and the $P^* - K_n^*$ plot shows a log-linear relationship with the slope of 1. This means that potential energy is proportional to mean stiffness coefficient $\widetilde{K}_n$ but slightly related to shear rate. At low concentration ($C = 0.40$), potential energy P^* decreases with the increase of K_n^* and the $P^* - K_n^*$ plot shows a log-linear relationship with the slope of $-1/2$. At medium concentration ($C = 0.58$), P^* is little affected by K_n^*. Figures 5(b), (d), and (f) clearly explain the corresponding relationship between potential energy and concentration. Potential energy has an increase tendency with the increase of concentration under different shear rates. Due to the different incremental rates and amplitudes, a crossing point appears at the concentration of $C = 0.58$. When $C < 0.58$, the faster the shear rates and the smaller the dimensionless stiffness K_n^*, the bigger the potential energy. When $C > 0.58$, the slower the shear rates and the bigger the dimensionless stiffness K_n^*, the bigger the potential energy. At medium concentration, there exists a critical value that could be used to clearly describe the critical point of the quasi-solid-liquid transition.

Quasi-solid-liquid transition can also be characterized by effective friction coefficient, contact time number, and coordination number (Babic et al. 1990; Campbell 2002, 2006). In fact, these parameters, although from a different point

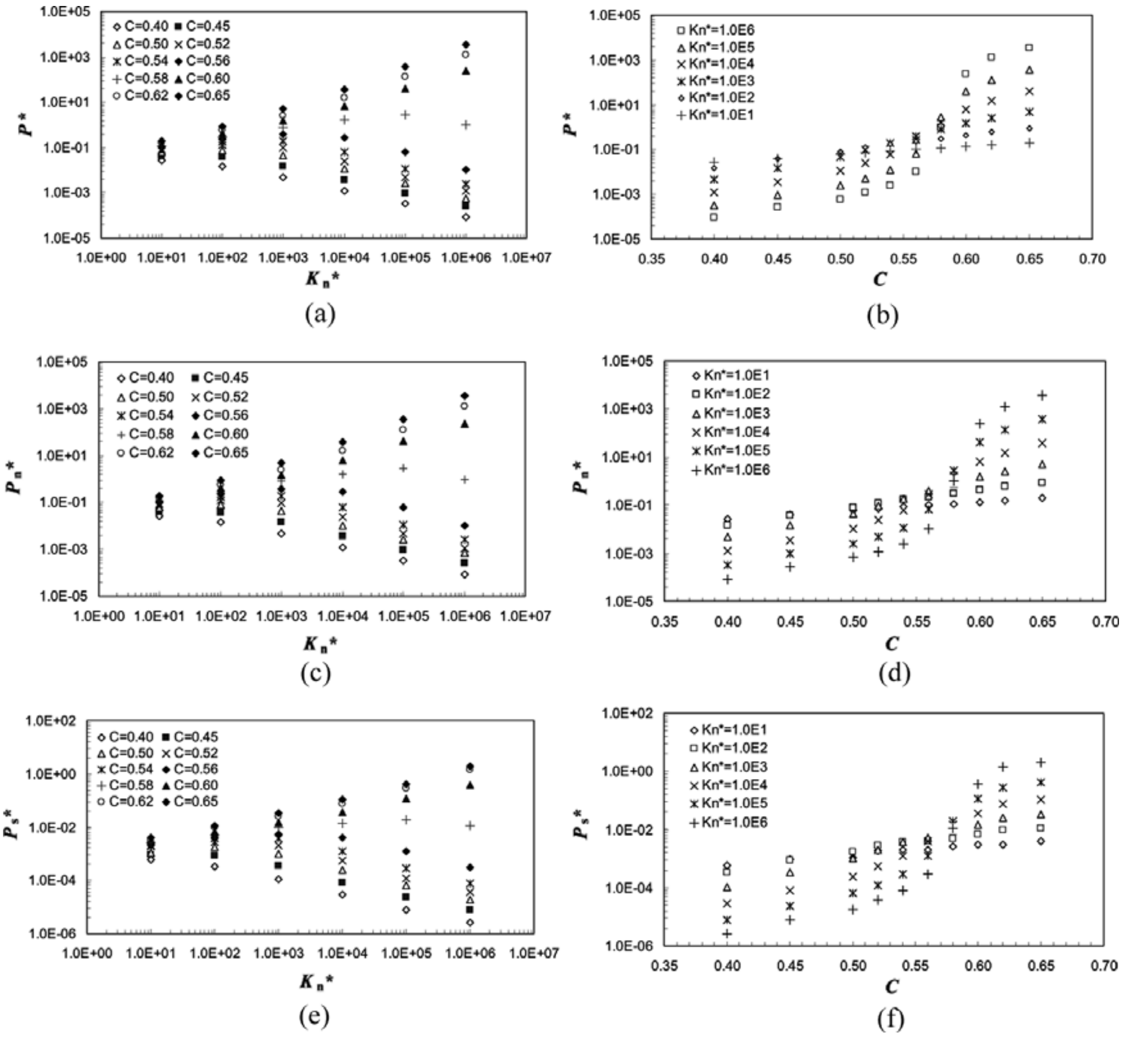

Figure 5. Elastic potential energy and its normal and tangential components of granular system under different shear rates and concentrations.

of view, reflect the same law of motion of granular media as elastic potential energy. For example, at low concentration, granular particles distribute dilutely and instant collisions are dominant. The frequency and intensity of collisions increase with the increase of shear rates. Macro-stress is proportional to the square of shear rates. Potential energy depends on collision intensity and frequency and is therefore proportional to shear rate. At high concentration, tight and persistent particle contacts come into being and relatively stable force chains form. With high coordination number, particle collision is controlled mainly by particle stiffness and deformation amplitude and is less related to shear rate. So, potential energy is determined by elastic deformation and particle stiffness and is independent of shear rate. At medium concentration, particle collision is in a critical state dynamically. The increase of shear rates accelerates the forming of new force chains and clumps and forces existing force chains to split and clumps to break up. The effective friction coefficient, contact time number, coordination number, and elastic potential energy can be kept at a relatively stable value. This is why there is a crossing point of elastic potential energy at the critical concentration as shown in Figure 5.

Through the above discussions, it can be concluded that energy distribution, especially elastic potential energy distribution, could be used to characterize the quasi-solid-liquid transition of granular media in steady state. The study of energy distribution in quasi-solid-liquid transition is helpful in combining the macro-statistics and micro-motion of granular media and in thoroughly understanding the dynamics of a granular system.

Conclusions

As a complex energy dissipative system, granular shear flow is an irreversible nonequilibrium process. To verify its energy conservation and determine energy distribution in quasi-solid-liquid transition in the steady state, a nonuniform granular system with periodic boundaries was simulated with the 3-D discrete element method. When the external power input just balances the internal energy dissipation rate, the granular system arrives at nonequilibrium steady state and energy is conserved. In view of energy fluctuations in the steady-state flow, fluctuations of force chains at microscale were investigated spatially and temporally. The effects of different parameters on energy distributions were then discussed. Finally, distribution of macro-stress and elastic potential energy were obtained and the quasi-solid-liquid transition point, which demarcates two distinct flow regimes, was identified. The consistency of using elastic potential energy or macro-stress, effective friction coefficient, coordination number, and contact time number were addressed in describing the phase transition of granular media. With the study of energy conservation and energy distribution in quasi-solid-liquid transition of granular system in nonequilibrium steady state, the intrinsic characteristics of granular materials can be understood deeply and rheology of granular media can be explored from the inherent energy viewpoint.

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