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Characteristics of temporal-spatial parameters in quasi-solid-fluid phase transition of granular materials

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Abstract The quasi-solid-fluid phase transition of granular materials is closely related to the shear rate and solid concentration in addition to their intrinsic properties. The contact duration and the coordination number are two important temporal-spatial parameters to describe the granular interaction in phase transition. In this study, characteristics of the contact duration and the coordination number associated with the transition processes are determined using a 3D discrete element model under different shear rates and concentrations. The resulting macroscopic stress and strain-rate relations are discussed. The temporal and spatial parameters provide a linkage between the macroscopic constitutive law and inter-particle micromechanics.

Keywords: granular flow dynamics, quasi-solid-fluid phase transition, coordination number, contact duration, macro-stress.

Granular materials are ubiquitous in agricultural and pharmaceutical processes, debris and snow avalanches, ice and sediment transport in rivers. A granular material can behave like a fluid when it flows or like a solid when it stops. It can transit between the two phases[1,2]. For example, beach sand can flow out of our fingers and fly with the wind. It can support our body weight when it lies on the ground. Ice floes can flow down the river. It can also form solid ice jam under proper condition. This solid-fluid phase transition for granular materials is a dynamic non-equilibrium process, and is usually called quasi-solid-liquid phase transition. The different constitutive behavior and the controlling factors in different phases are important problems in current studies of granular materials. A number of physical experiments, theoretical analyses and numerical simulations have been performed to investigate the characteristics of quasi-solid-liquid phase transition to establish constitutive models for granular materials[3−5].

Macroscopic dynamic properties of granular materials are closely related to the particle scale micromechanics, and their statistical characteristics. In a dense flowing granular material, colliding particles form clusters. Force chains form in these clusters transmit load. These force chains serve as an important index of the strength of a granular material[6]. The contact duration between colliding particles and the coordination number are two important parameters to describe the time-space characteristics of the force chain. When uniform size particles are packed in a hexagonal pattern, the concentration reaches it maximum at 74.05%. The corresponding coordination number is at its largest value of 12, and the contact time can be infinitely long. As such, the granular material behaves as a solid. With a decrease in the concentration and an increase in the shear rate, some force chains break. Both the coordination number and the contact duration decrease. When the concentration becomes sufficiently low, the force chains cease to exist. The coordination number and the contact duration approach 0 and the binary contact duration T_{bc}, respectively. In this case the granular material resembles a fluid. During the phase transition described above, the macro-stresses change from rate-independent to rate-dependent. In the physical experiments of granular flow dynamics, such as flow over an inclined surface, within a shear cell, a rotating cylinder, or inside a channel, the macroscopic parameters such as velocity distributions, shear rates and stress fields, have been measured directly or indirectly to demonstrate the quasi-solid-liquid phase transition[7−10]. However, due to the difficulty in measuring the micro-parameters such as the contact duration, the coordination number and the contact force, the phase transition of granular materials with different concentrations and shear rates cannot be determined systematically by using physical experiments. Therefore, discrete element models have been adopted widely to study granular flow dynamics[11−13]. In this study, a 3D simple shear granular flow with periodic boundaries is simulated. Based on the simulation results, the temporal-spatial parameters, i.e. the contact duration and the coordination number, are determined to characterize the quasi-solid-liquid phase transition.

1 Numerical model of granular flow dynamics

The discrete element model (DEM) for granular materials was established in the 1970s. Over the last few decades this method has been improved to such an extent that many real physical processes involving granular materials can be realistically simulated. A DEM algorithm includes the initial packing, the search routine, the contact force model, the motion integration, statistical averaging for the velocity field, macro-stresses and strains, and the energy balance of granular systems[14]. Using the DEM simulation as a numerical experiment, many interesting phenomena of the dynamic behavior of granular materials have been discovered. In this study we use DEM to analyze phase transition in granular materials. In the section below we briefly introduce several crucial quantities in this study: the contact force model, macro-stresses, the contact duration, and the coordination number.

1.1 Contact force model for granular collisions

The intrinsic properties of granular materials and the physical contact process are two most important factors in establishing the contact force models. In dry granular materials, the contact force among particles can be modeled using a viscous-elastic model with friction sliding. Such a contact law allows the bulk material to behave according to a Mohr-Coulomb friction law. This viscous-elastic model can be either linear or nonlinear. Theoretically, the Hertz-Mindlin nonlinear model is more accurate in simulating the physical collision between elastic bodies. But the linear model is more convenient to simulate the granular flow dynamics in quasi-solid-liquid phase transition, and the simulated results are qualitatively insensitive to the choice between linear and nonlinear contact laws[4,11,13].

The viscous-elastic contact force model is shown in Fig. 1. Here the normal and tangential stiffness and damping coefficients have the relationship of $K_s = \alpha K_n$, $C_s = \beta C_n$, where α = 0.8 or 1.0, β = 0.0[4,11,13]. The normal damping coefficient can be calculated as

$$C_n = \zeta_n \sqrt{2MK_n}\,, \tag{1}$$

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

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

In the linear viscous-elastic contact force model, the binary contact time of a pair of isolated colliding particles can be calculated as

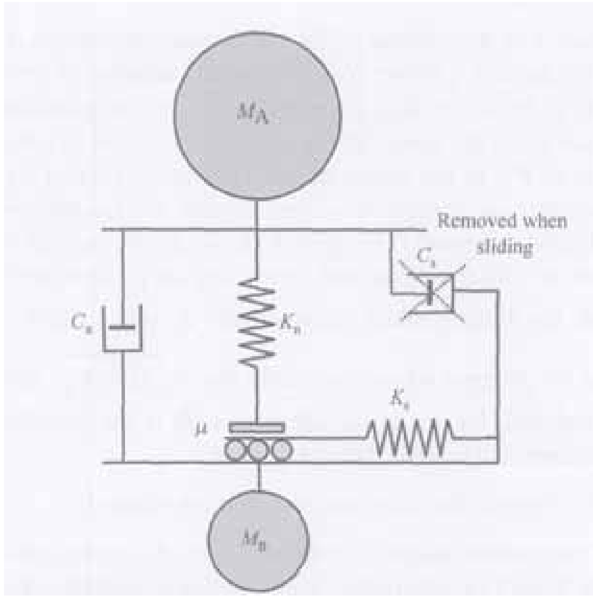

Fig. 1. Contact force model for granular collision. M_A and M_B are the mass of particles A and B, K_n and K_s are the normal and tangential stiffness, C_n and C_s are the normal and tangential damping coefficients, μ is the friction coefficient.

$$T_{bc} = \frac{\pi}{\sqrt{\frac{2K_n}{M}(1-\zeta_n^2)}}\,. \tag{3}$$

This duration is called the "binary contact time". In the linear force model, this duration is a constant determined by the particle size and material properties, and can be used to describe the granular flow characteristics. In the numerical simulation of granular flow, the computational time step is usually set at 1/50 of the binary contact time.

1.2 Macro-stresses in granular materials

By numerically simulate the particle contact process of granular materials at a micro-scale, the contact force and fluctuation velocity of each particle can be determined. Through statistically averaging the particle level information we may determine the macro-stresses. The macro-stresses consist of the contact stress and the kinetic stress, and can be expressed as

$$\sigma_{ij} = \sigma_{ij}^{c} + \sigma_{ij}^{k}\,, \tag{4}$$

where σ_{ij} is the macro-stress, σ_{ij}^{c} and σ_{ij}^{k} are the contact stress and the kinetic stress. And we have

$$\sigma_{ij}^{c} = \frac{1}{V}\sum_{k=1}^{N}\sum_{l=1}^{N_k}(r_i^{lk} F_j^{kl})\,, \tag{5}$$

$$\sigma_{ij}^{k} = \frac{1}{V}\sum_{k=1}^{N} M_k (u_i'^{k} u_j'^{k})\,, \tag{6}$$

where V is the volume of the computational domain, N is the particle number, N_k is the contact number of 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_i^{kl} is the tensor of the total force exerted by particle l on particle k, $u_i'^k$ and $u_j'^k$ are the fluctuation velocity components of particle k. To study the influence of concentrations and shear rates on phase transition, the dimensionless macro-stress $\sigma_{ij}^* = \sigma_{ij} / \rho D^2 \gamma^2$ and the dimensionless shear rate $B = \gamma \sqrt{\rho D^3 / K_n}$ are introduced. Here γ is the shear rate, D is the particle diameter, and ρ is the particle density.

1.3 Contact duration and coordination number

The contact duration is the duration of a given contact, binary or otherwise. When multiple particles are engaged in a collision, the contact time for any pair within this cluster may be shorter or longer than the collision of an isolated pair. We define a dimensionless contact duration called the contact time number m. The contact time number is the ratio of the mean contact duration to the binary contact time T_{bc}, written as

$$m = \frac{\overline{T}_c}{T_{bc}}. \quad (7)$$

The binary contact time T_{bc} is a constant based on the material property. Therefore, the contact time number is an effective index for a granular flow to measure the mean contact time as a function of the kinematics alone.

In granular flow dynamics, the coordination number is defined as the average number of contacts per particle,

$$n = \frac{\sum_{k=1}^{N} n_c^k}{N}, \quad (8)$$

where n is the coordination number, n_c^k is the contact number of particle k and N is the total number of particles.

2 Numerical simulation of phase transition for granular materials

In this study the linear viscous-elastic contact force model is adopted to simulate the granular dynamic process with a 3D DEM using uniform spheres. Periodic boundary conditions are used to generate a simple shear flow. The resulting macro-stresses, contact time number and the coordination number are discussed.

2.1 Initial packing, sample size and boundary conditions of granular materials

Using DEM to simulate granular flow dynamics the initial packing of granular materials can be regular or random. It is straightforward to achieve a dense packing up to the highest concentration for uniform-size granular materials if regular packing is used. For multi-size granular materials, especially those with large variations in diameter sizes, random packing is required to obtain dense concentration. In this study, although uniform size granular materials are used, a random packing pattern is also adopted to make the granular materials reach the dynamical equilibrium, and to study its random statistic properties within a shorter initialization time. In order to overcome the difficulty in dense packing with random patterns, the computational domain is filled randomly with small particles first, and then the particles are allowed to swell to their required sizes. The regular packing patterns by hexagonal close packed (HCP) and face centered cubic (FCC) are shown in Fig. 2(a) and (b). The random-growth packing for single-size and multi-size particles are shown in

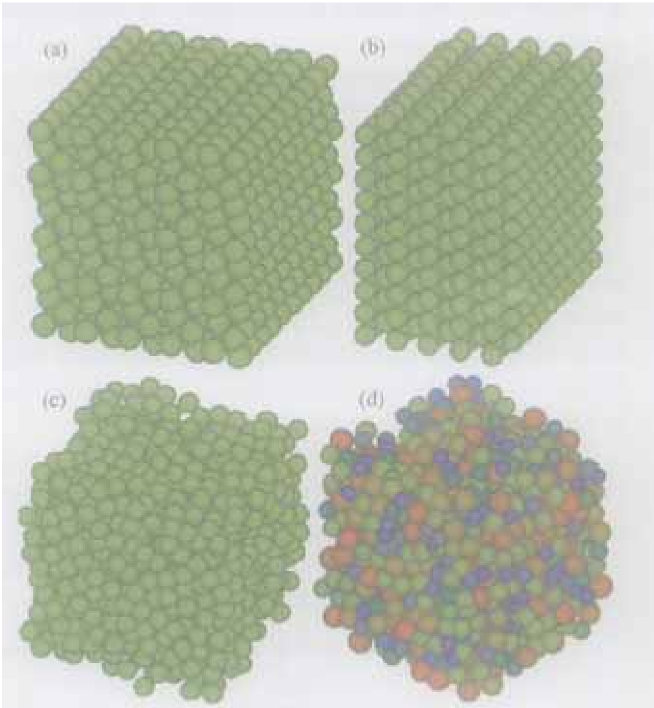

Fig. 2. Initial packing patterns of granular material. (a) Hexagonal close packed (HCP); (b) face centered cubic (FCC); (c) random packing for uniform size granular; (d) random packing for multi-size granular. In (a) and (b), the concentration is C = 0.6 and the particle number is 10×10× 10. In (c) and (d), the concentration is C = 0.6 and the computational domain is $10\tilde{D} \times 10\tilde{D} \times 10\tilde{D}$, here $\tilde{D}$ is the mean particle diameter.

Fig. 2(c) and (d).

To model the continuous shear flow of granular materials with different concentrations and shear rates, we adopt the periodic boundary condition. The periodic boundary is similar to that of the granular flow in a Couette shear cell, and is used in the study of granular flow dynamics widely[4,11,13]. The granular material has a shear rate of $\gamma = U/b$ in y direction, and has a random fluctuation in x and z directions. Here U is the relative velocity between the top and the bottom boundary. When particles flow out from one side, they re-enter from the opposite side to keep the total mass and concentration conserved.

In the computation of granular shear flow dynamics, the boundary resistance will affect the simulated results greatly if the computational domain is too small. The low computational efficiency is the shortcoming of DEM. The computational cost will increase sharply with the increase in the domain size[15]. Therefore, it is necessary to determine a reasonable domain size. In this study, it is found that the boundary influence could be avoided when the computational domain is at least $a \times b \times c = 10D \times 10D \times 10D$[13].

With the above initial packing pattern, boundary condition and computational domain size, the granular shear flow dynamics is simulated using DEM. The main parameters are listed in Table 1. The physical units of these parameters are set at unity to analyze the dimensionless results conveniently.

Table 1 Parameters in shear flow simulation

Definition	Value	Definition	Value
Particle diameter	$D = 1.0$	Restitution coefficient	$e = 0.7$
Density	$\rho = 1.0$	Friction coefficient	$\mu = 0.5$

2.2 Macro-stress

The flow dynamics are simulated at different concentrations and shear rates. In the simulated dimensionless macro-stress $\sigma_{ij}^* = \sigma_{ij} / \rho D^2 \gamma^2$, the shear σ_{12}^* and normal stress σ_{22}^* in the x-y plane are plotted in Fig. 3. The other stress components σ_{11}^* and σ_{33}^* have similar distributions to σ_{12}^* and σ_{22}^*. If the granular flow is roughly divided into three states, namely rapid flow, slow flow and quasi-static state based on its dynamic behavior, their flow properties and quasi-solid-liquid phase transition can be obtained from the simulated results.

Fig. 3(a) and (b) shows that the dimensionless macro-stress $\sigma_{ij}^* (= \sigma_{ij} / \rho D^2 \gamma^2)$ is independent of the dimensionless shear rate $B = \gamma \sqrt{\rho D^3 / K_n}$ at low concentration (C = 0.40), suggesting that the macro-stress σ_{ij} does not have any relationship with material stiffness K_n, but it is proportional to the square of shear rate γ. In this situation, the granular material

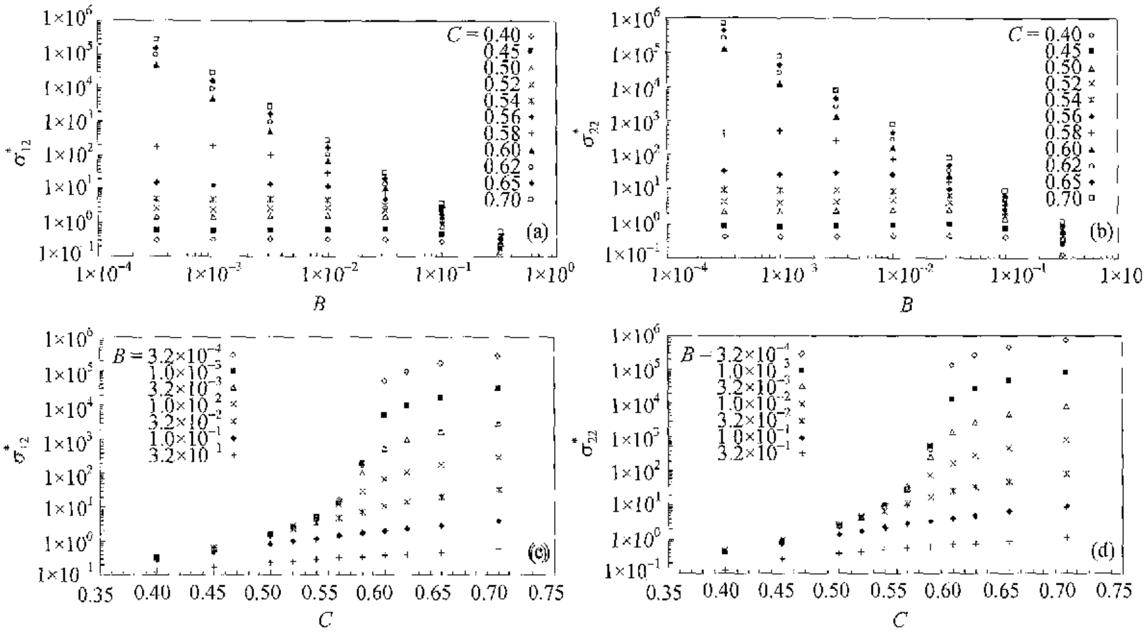

Fig. 3. Macro-stress versus concentration and shear rate. Here the dimensionless shear rate $B = \gamma \sqrt{\rho D^3 / K_n}$.

appears as a rapid flow, and has the properties of a fluid. At high concentration ($C > 0.60$), σ^*_{ij} is a linear function of B with exponential slope -2. This means that the macro-stress σ_{ij} is independent of the shear rate γ, but has a linear relationship with stiffness K_n. In this situation, the granular material lies in the quasi-steady sate, and has the properties of a solid. At an intermediate concentration of C = 0.58, σ^*_{ij} is independent of B at slow shear rate, and has a linear relationship with B at fast shear rates. This means that the granular material changes from quasi-static flow to rapid flow when B is slowed down, and the granular material exhibits a phase transition from a quasi-solid to a fluid.

To analyze the influence of concentration, the simulated macro-stress is plotted in Fig. 3(c) and (d) with respect to C. At high shear rate, σ^*_{ij} increases slowly with an increase in shear rate. With a decrease in shear rate B, the influence of concentration on σ^*_{ij} becomes more and more obvious, and σ^*_{ij} increases drastically beyond C = 0.58. Therefore, the granular material resembles a quasi-static flow or rapid flow at high or low concentrations, respectively, and exhibits various flow states at medium concentrations according to different shear rates.

Shen *et al*. and Campbell obtained similar distributions of macro-stress with 2D and 3D DEM simulations, independently, and also discussed the phase transition from the rapid flow dominated by inertial collisions to the quasi-steady state dominated by elastic contacts[11,13]. In the following, the characteristics of a phase transition will be discussed in terms of the simulated contact time number and coordination number.

2.3 Contact time number

The contact time number is the ratio of mean contact time to binary contact time. This parameter describes the duration of force chain from generation to breakup. In a single collision between two isolated particles, the contact time is the binary contact time T_{bc}, and its contact time number m = 1. In multi-particle-collisions, the contact time is altered due to the action with other particles. Occasionally the duration of a given collision may be shortened from the binary contact time if a pair of colliding particles is hit by a third one opposite to their interaction. But normally, the mean contact time number $m > 1$ when multiple contacts persist. Subtract the binary contact time from the collision time. Then the net contact time number m' (= m−1) can be used to describe the influence of the extended contact in multi-collisions.

The contact time number m and the net contact time number m' (= m−1) are plotted in Fig. 4. From Fig. 4(a) and (b), it is observed that the net contact time number approaches zero at low concentrations and low shear rates. When the shear rate increases keeping the same low concentration, the net contact time number in-

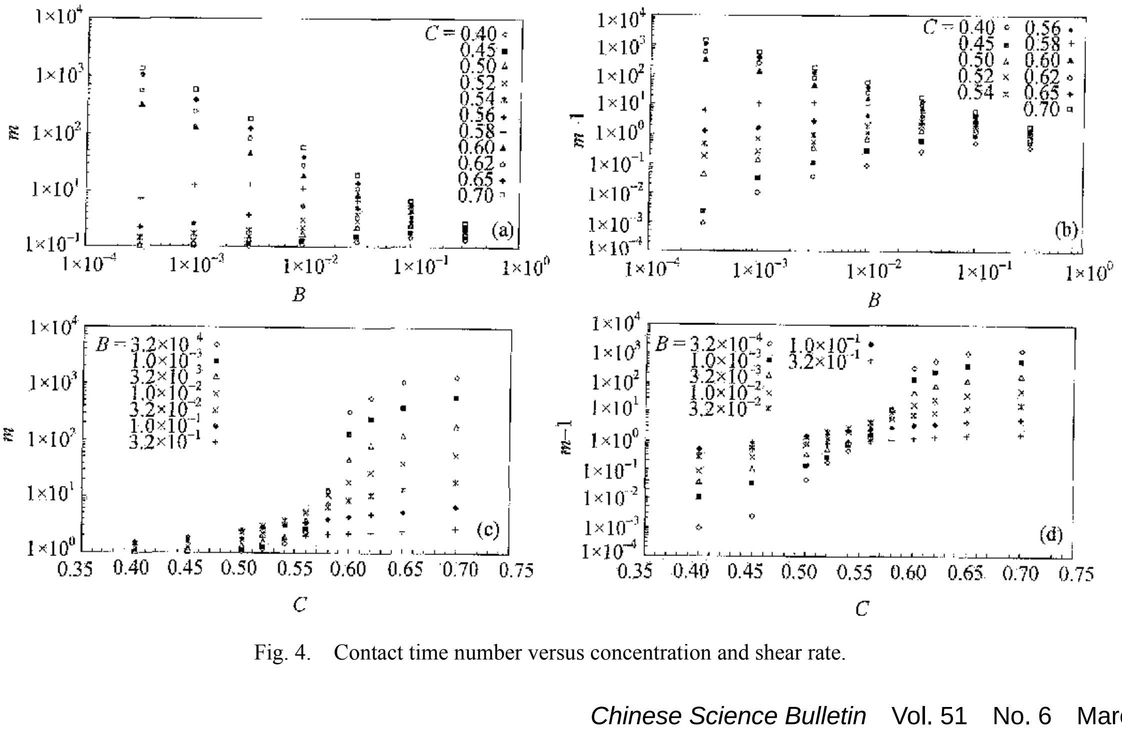

Fig. 4. Contact time number versus concentration and shear rate.

creases and approaches the binary contact time. The contact time number has the largest value that exceeds 10^3 at high concentrations and slow shear rates. At high concentrations when the shear rate increases the net contact time number decreases, and interestingly approaches the binary contact time as well.

When the contact time is long, the force chains are persistent. Thus the granular material appears as in a quasi-static state at high concentrations and slow shear rates. On the other hand, when most of the collisions are binary, the force chains break easily. This happens at low concentrations for a wide range of shear rates. In rapid flow conditions with high shear rates, the contact time number is not as closely related with concentration as at the low shear case. In the rapid shear state, the granular material lies in a dynamic state with high frequency random collision and formation and breakage of clusters.

From Fig. 4(c) and (d), an interesting phenomenon is observed. The net contact time number m' has a cross-over at the concentration about C = 0.56. If C < 0.56, the contact time increases with increasing shear rate. On the other hand, if C > 0.56, the contact time increases with decreasing shear rate. This phenomenon suggests that the concentration is the principal factor that affects the generation and breakup of force chains, and the force transition and distribution. Therefore, we introduce this critical concentration C^* = 0.56 as a characteristic number for phase transition. Around this concentration, the contact time number is around m^* = 2.0 independent of the shear rate. When $C > C^*$, we have $m > m^*$, and the granular material appears as in the quasi-static state; when $C < C^*$, we have $m < m^*$, and the granular material appears as in a fluid state; when C is around C^*, we have $m \rightarrow m^*$, and the granular flow performs a phase transition at different shear rates for each different C. The contact time number m can thus serve as a characteristic parameter to determine the phase of granular materials.

2.4 *Coordination number*

The coordination number is the mean contact number of a particle. It can express the force chain distribution spatially, and has a close relationship with the macro-stress and the contact time number. The simulated coordination number versus concentration and shear rate is shown in Fig. 5.

From Fig. 5(a), we can find that the coordination number increases with an increase in the shear rate at

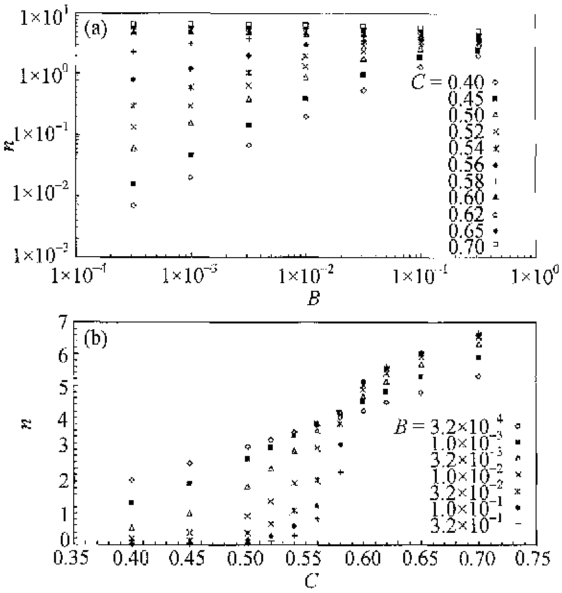

Fig. 5. Coordination number versus concentration and shear rate.

low concentrations, and decreases with an increases in shear rate at high concentrations. When the coordination number approaches zero, contact between particles is rare. The granular material flies freely. This state is realized at low concentration and slow shear rate. At high concentration but slow shear rate, as the concentration increases the coordination number also increases until the granular materials reaches the quasi-static state. At high shear rates or under the rapid flow condition, the coordination number has weak relationship with the concentration. From Fig. 5(b), we can also see that the coordination number increases with the increase of concentration, but the slope is steeper at slow shear rates.

The distribution of coordination number at different concentrations and shear rates is also similar to that of contact time number. The coordination number decreases with the increase in shear rate at high concentration, and with the decrease in shear rate at low concentration. At an intermediate concentration (C = 0.59), the coordination number is independent of the shear rate, and keeps around a constant value of n^*=4.0. Ball and Blumenfeld discussed the analytical coordination number based on the dynamic equilibrium mechanism, and found that the critical number is 4 and 6 for rough and smooth granular materials, respectively[16]. In the present simulation of rough granular materials with a contact friction of μ = 0.5, the simulated critical coordination number is 4, which is consistent with the analytical number.

From the above analysis, $n^* = 4.0$ appears to be another candidate for the phase transition of a granular material. If $n < n^*$, the granular material is rate-dependent and in a state of a fluid. If $n > n^*$, the granular material is in a quasi-static state, and appears as a solid material. If n is around n^*, the granular material has an intermediate concentration around $C^* = 0.59$, and phase transition occurs at a different shear rate for each different C.

3 Phase transition described with contact time number and coordination number

The phase transition and its micro-, macro-mechanical properties should be determined first in order to study the constitutive model in quasi-solid-fluid transition. In the process from rapid to slow and finally quasi-static flow, the granular phase is determined by the rate-dependency of the macro-stress on the shear rate[4,11,13,17,18]. The granular material appears as a non-Newtonian fluid and can be modeled by the kinetic theory with granular temperature when the macro-stress increases linearly with the square of shear rate. The granular material appears as in the quasi-static state and can be modeled by the plastic theory when the macro-stress is independent of the shear rate. The constitutive law within the phase transition zone is an open question[1,9,13,17,18].

Based on the numerical results simulated using 2D discrete element model, Babic et al. qualitatively discussed the phase transition from rapid to slow and finally quasi-static flow under different concentrations and shear rates (Fig. 6, the dimensionless shear rate $B^* = \gamma\sqrt{M / K_n}$). In the transitional zone A, binary collisions in granular rapid flow change to multi-collisions, and some force chains appear, but they are very weak and can be broken easily. In transition zone B from slow flow to quasi-static state, steady clusters appear in the granular material, and the force chains are quite strong and cannot be broken easily[17]. Recently, Campbell also obtained similar transitional properties as shown in Fig.6 via numerical simulations using 3D DEM[13]. In some physical experiments, transitions between dilute-dense flow and dense flow-jam can occur[10,19]. These flow transitions are very similar to the phase transition from rapid flow to slow flow and quasi-static state.

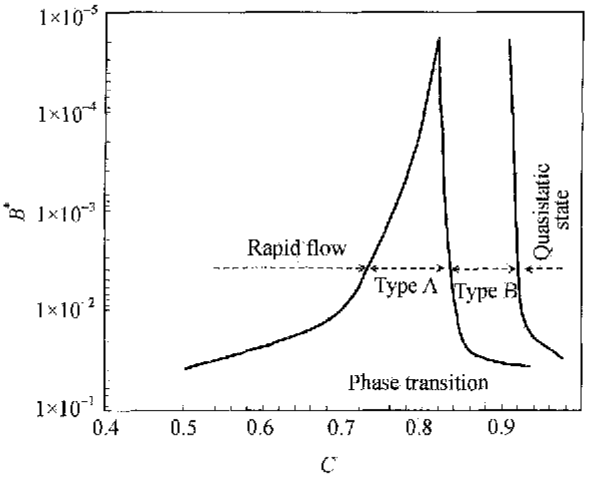

Fig. 6. Phase transition from rapid flow to quasi-static flow in 2D granular flow material[17].

In the phase transition of quasi-solid-fluid, the contact time number and the coordination number can directly describe the formation and break of force chain, cluster and aggregation of particles. To analyze the phase transition of granular materials, the net contact time number m' (= $m-1$) and the coordination number n, are plotted in 2D and 3D contours versus concentration C and shear rate B (as shown in Figs. 7 and 8). The basic characteristics shown in Figs. 4 and 5, associated with the phase transition process can also be displayed in these contour plots. In addition, these contour plots more clearly depict the phenomena shown in Fig. 6. At low concentrations, the contact time number and the coordination number are smaller than their critical number $m^* = 2.0$ (i.e. $m' = 1.0$) and $n^* = 4.0$ respectively, and increases as the shear rate drops. At high concentration, both the contact time and the coordination number are larger than m^* and n^* respectively, and they increase when the shear rate is faster. The phenomena above can be explained as follows. In a rapid flow with low concentrations, the granular flow has low contact frequency and short contact time, and the number of particles in a cluster is also very small. As the shear rate increases, the particle movement becomes more intensive. The increase of contact frequency accelerates the generation of force chain. In the quasi-static state with high concentration, the granular force chain is persistent, but some force chains are broken with the increase of shear rate. As a result, the particles disengage from clusters, which can reduce the contact time and the coordination number. For intermediate concentrations, the granular flow and its interaction keep a dynamic balance. With the increase of shear rate, some of the existing force chains are broken with some new ones generated. In this way, the contact time and the coordination number are kept constant.

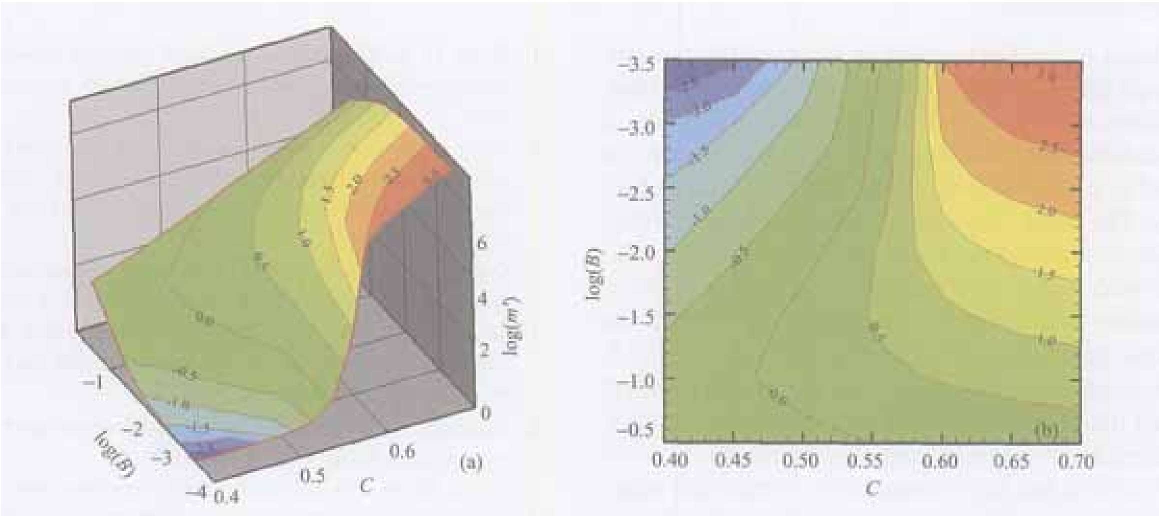

Fig. 7. Contour of the log of net contact time number log(m') in phase transition of granular material.

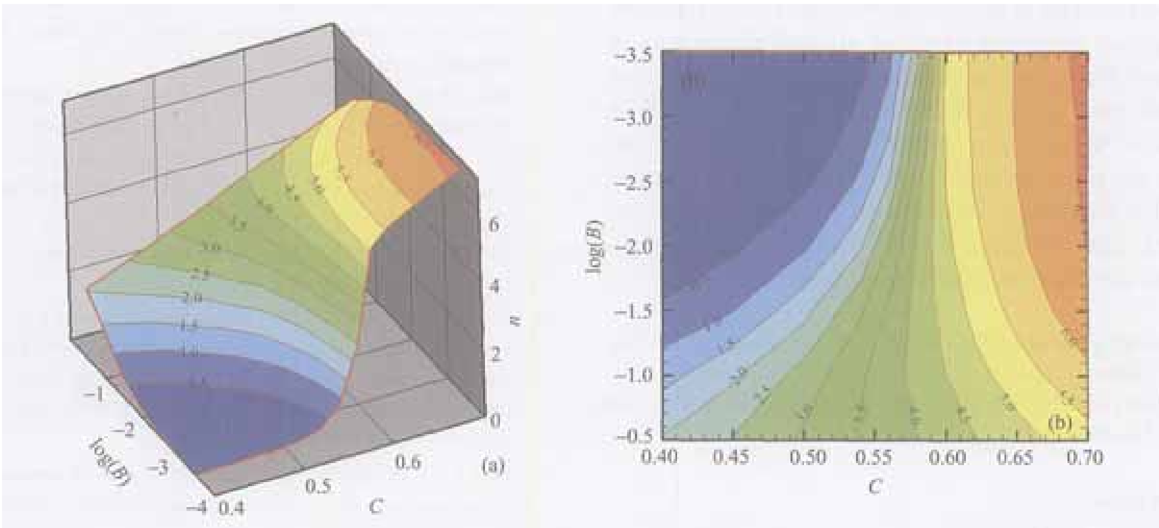

Fig. 8. Contour of coordination number in granular phase transition.

From Figs. 4 and 5, we can find the critical contact time number $m^* = 2.0$ and the critical coordination number $n^* = 4.0$ corresponding to concentrations C = 0.56 and 0.59, respectively. These critical numbers can be used to identify the granular phase. Considering the difference in the concentrations for m^* and n^*, the contours of the net contact time and the coordination numbers in Figs. 7 and 8, and the phase transitional process in Fig. 6, we conclude that there is an intermediate concentration zone, i.e. $C \in [0.56, 0.59]$, for granular phase transition. In this intermediate zone, both the contact time number and the coordination number approach their critical values when granular flow changes from rapid to slow flow with increasing C or from quasi-static to slow flow from a decreasing C. At low shear rates, the transition process is obviously faster from Figs. 7 and 8. The stress state can be used to determine the granular phase properties and interior strength (Fig. 3).

4 Conclusions

The phase transition from rapid to slow flow and eventually to the quasi-static state is studied at different concentrations and shear rates based on the results of a 3D DEM simulation of uniform spheres under the simple shear condition. The flow properties in these three phases are discussed in terms of the simulated macro-stress, contact time number and the coordination number. The contact time number and the coordination number can be used to infer the temporal-spatial characteristics of the force chains in the granular material. Through the relationship between contact time number, coordination number and concentration, shear rate, it was demonstrated that the granular material appears as a fluid or a solid at low or high concentration, respectively. The phase transition occurs at a range of intermediate concentration. Based on the numerical results, the critical contact time number m^* and the critical coordination number n^* are introduced to identify the granular flow phase. If the friction coefficient $\mu = 0.5$, and restitution coefficient $e = 0.7$, we have the critical contact time number $m^* = 2.0$ and the critical coordination number $n^* = 4.0$ at the intermediate concentrations of $C^* = 0.56$ and 0.59, respectively. Within this range of concentration, the granular material transitions from slow flow to rapid flow at low concentration, and to quasi-static state at high concentration. The quasi-solid-fluid phase transition exists in all granular materials, but their critical contact time number and coordination number vary with different material properties. With the aid of contact time number and coordination number in the phase transition, the rehological behavior of granular materials in different phases can be better explained. These insights will be helpful to the establishment of the macro-constitutive models.

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