Rheology of cohesive granular materials

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Using molecular dynamics simulations, we study the plane shear flow of an assembly of slightly polydisperse disks, at controlled pressure and shear rate, without gravity. We use biperiodic boundary conditions to avoid wall perturbations. We add to the usual interaction term (elasticity, friction and dissipation) a cohesive force of the Van der Waals type. The properties of this system depend on two dimensionless numbers. The first one is related to the shear state imposed to the material. The second one characterizes the intensity of the cohesion. In steady homogeneous shear flows, we measure the variations of the solid fraction and of the effective friction as a function of those two numbers, from which we deduce a viscoplastic constitutive law. Moreover, the grains agglomerates in transient clusters when the cohesion number increases. The analysis of the space and time correlations shows a structural transition when the cohesion force becomes larger than the confinement force.

1 INTRODUCTION

Dense flows of cohesionless granular materials have been recently the focus of various experimental and numerical studies (GDR MIDI 2004). Within the simple plane shear geometry, with prescribed pressure and shear rate, it was possible to identify the constitutive law, that is to say the dependency of the stress components on the shear rate (da Cruz et al. 2005). In particular, the integration of the friction law in Saint-Venant codes allows large scale simulations of granular flows (Pouliquen and Forterre 2002; Naaim et al. 2004).

However, in various granular materials such as snow (Bouchet et al. 2003), humid grains (Tegzes et al. 2002) or powders (Castellanos et al. 1999), cohesion forces between grains can not be neglected. Discrete numerical simulations give access to the influence of these forces on the rheology of an assembly of grains (Mei et al. 2000; Nase et al. 2001; Iordanoff et al. 2005). In this paper, we present the simulation of the plane shear flow of an assembly of cohesive grains. We first identify the two parameters controlling the simulated system : the shear state and the cohesion intensity. Then we measure the dependencies of the constitutive law on the cohesion intensity. Last, we relate those macroscopic observations to the evolution of the microstructure.

2 SIMULATED SYSTEM

The granular material is a two dimensional assembly of disks of average diameter d and average mass m. A small polydispersity (20%) is introduced to prevent crystallization. It is submitted to plane shear, without gravity, so that the stress distribution is uniform. Both shear rate $\dot{\gamma}$ and pressure P are prescribed by bi-periodic boundary conditions (Radjai and Roux 2002; Gilabert et al. 2005) (Fig.1). The use of these boundary conditions avoids wall perturbations (Iordanoff et al. 2005). The shear cell (height H, length L) is repeated periodically along the two directions. The control of the pressure P is achieved by allowing the expansion of the shear cell along y : the evolution of H is given by : $\dot{H} = (P - P_0)L/g_P$, where g_P is a viscous damping parameter, and P_0 is the average pressure in the shear cell. Steady state corresponds to $\langle P_0 \rangle = P$. The top and bottom cells move with a velocity $\pm V(t)$, which is adapted to maintain a constant shear rate : $\dot{\gamma} = V(t)/H(t)$. The granular shear state is controlled by a single dimensionless I, parameter called inertial number (da Cruz et al. 2005), ratio of

inertial to shear times :

$$I = \dot{\gamma}\sqrt{\frac{m}{P}}. \quad (1)$$

In this paper we focus on the dense regime ($I \in [0.025\ ;\ 0.3]$), where the contact network percolates through the cell.

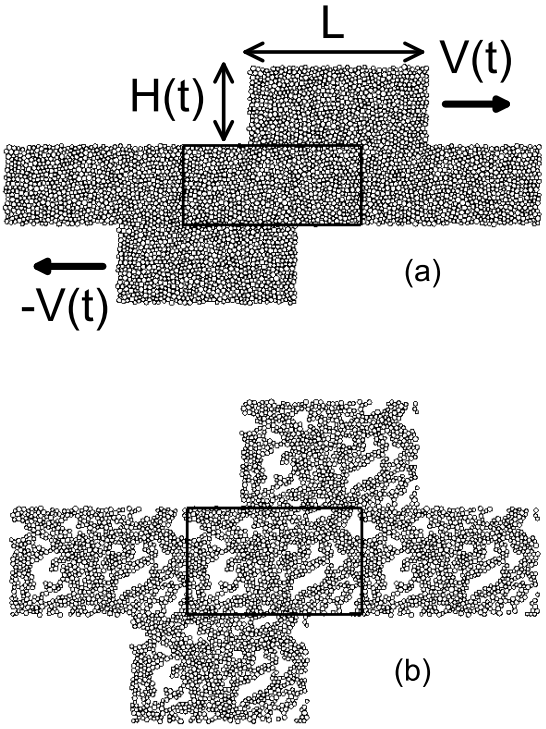


FIG. 1. Bi-periodic boundary condition ($I = 0.1$).(a) $\eta = 0$, (b) $\eta = 2$.

The shear is simulated by standard molecular dynamics method adapted to granular materials (Roux and Chevoir 2005). The contacts are visco-elastic (stiffness k_n and viscosity g_n), frictional (friction coefficient μ) and cohesive. The cohesion force is a normal van der Waals type force, equal to the product of the interfacial energy γ and the contact area (length in two dimension) (Matuttis and Schinner 2001; Preechawuttipong 2002). The total normal force f_n is a function of the normal interpenetration h : $f_n = k_n h + g_n \dot{h} - \gamma\sqrt{2hd}$. According to previous parametric studies (da Cruz et al. 2005), k_n, g_n and μ have a very small influence on cohesionless grain flows. We shall assume this holds for cohesive grain flows. The simulations presented in this paper were done with $\mu = 0.4$ and $g_n = 10^2$ (corresponding to a restitution coefficient of 0.1 in a binary collision). Moreover, we chose $k_n/P = 10^4$, which corresponds to the limit of rigid grains.

With this cohesion model, the maximum traction force is $F_c = \frac{\gamma^2 d}{2k_n}$. We introduce a dimensionless cohesion number η as the ratio of F_c over the typical confining force Pd :

$$\eta = \frac{\gamma^2}{2k_n P}. \quad (2)$$

This dimensional analysis predicts a regime of low cohesion when $\eta \leq 1$ and a regime of a high cohesion when $\eta \geq 1$ ($\eta = 0$ corresponds to cohesionless grains).

The grains are randomly deposited without contact in the shear cell. Then pressure P and shear rate $\dot{\gamma}$ are imposed. After a sufficient amount of time, the flow reaches a steady homogeneous shear state, which does not depend on the initial configuration, characterized by constant time-averaged solid fraction ν, shear rate and stress tensor. We measure the macroscopic constitutive law and the microstructure in those steady flows.

3 CONSTITUTIVE LAW

We call "dilatancy law" the variations of the solid fraction as a function of I and η (Fig.2 (a)). ν decreases approximately linearly with I, starting from a maximum value ν_{max} :

$$\nu(I, \eta) \simeq \nu_{max}(\eta) - aI. \quad (3)$$

ν_{max} strongly depends on the cohesion number η : $\nu_{max}(\eta) \simeq 0.81 - 0.03\eta$ while the slope a varies slowly with η.

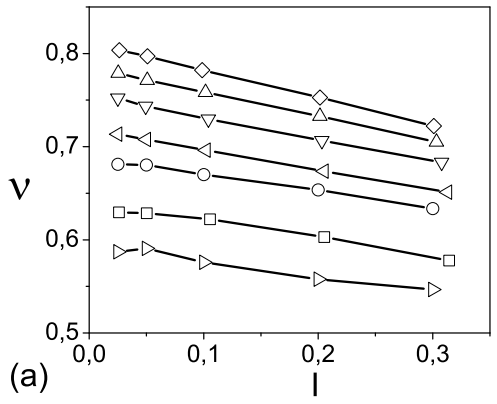
We call "friction law" the variations of the effective friction coefficient μ^* (ratio of the shear stress S to the pressure P) as a function of I and η (Fig.2 (b)). For small cohesion ($\eta \leq 1$), μ^* increases approximately linearly with I, starting from a minimum value μ^*_{min} :

$$\mu^*(I, \eta) \simeq \mu^*_{min}(\eta) + bI. \quad (4)$$

For $\eta \leq 1$, μ^*_{min} and b are nearly constant. For larger cohesion, we first observe a sudden increase of μ^*_{min}, for η between 1 and 2. Then, for $\eta \geq 3$, the effective friction increases again, but the friction law (Eqn. (4)) is no more valid.

For small cohesion ($\eta \leq 1$), those measurements generalize what has been observed in cohesionless granular materials (da Cruz et al. 2005). Then, from the dilatancy and friction laws, it is possible to deduce a visco-plastic constitutive law. But they evidence a transition of behavior, above a critical cohesion number $\eta \simeq 1$, in agreement with the prediction of dimensional analysis. Such a transition was observed by Iordanoff et al. (2005) in a confined layer. However, we

notice that this transition is not apparent on the dilatancy law. We shall now interpret this transition on the basis of microstructural observations.



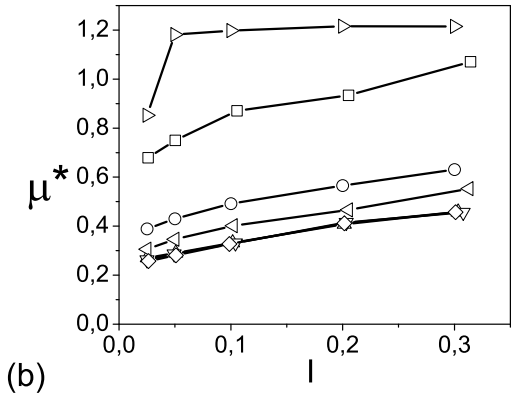


FIG. 2. (a) Dilatancy law, (b) friction law. η = 0($\diamond$) ; 0.2 ($\triangle$) ; 0.5($\bigtriangledown$) ; 1($\triangleleft$) ; 1.5($\circ$) ; 2 ($\square$) ; 3 ($\triangleright$)

4 MICROSTRUCTURE

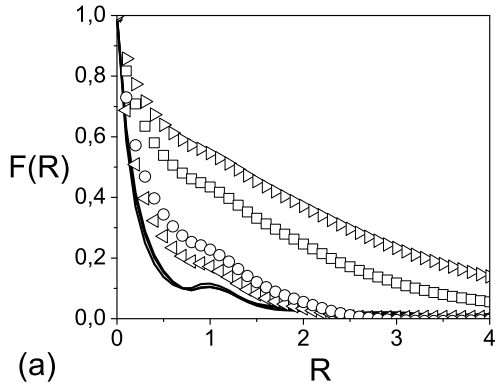
Fig.1 (b) shows that as the cohesion increases, the granular material becomes more heterogeneous, and is made of dense clusters separated by voids. This point was also observed in ref. Mei et al. (2000). Consequently, the average solid fraction is decreasing as the granular material is becoming more porous. For a very strong cohesion ($\eta \geq 3$), the material is fractured in two parts. As a way to characterize quantitatively the increasing heterogeneity of the granular material, we now present measurements of space and time correlations.

4.1 Spatial heterogeneity

At each time step, we perform a radical tesselation (Annic et al. 1994) : the Voronoï polygone around each grain corresponds to the points which are closer from this grain than from any other grain. Then, the local solid fraction around each grain is defined as the ratio of the areas of the grain and of its Voronoï cell. This defines the field of solid fraction $\nu(\vec{r})$. The characteristic length scale of the heterogeinities (both clusters and voids) is deduced from the autocorrelation $F(\vec{R})$ of the fluctuating solid fraction field $\delta\nu(\vec{r})$:

$$F(\vec{R}) = \frac{\langle \delta\nu(\vec{r})\delta\nu(\vec{r}+\vec{R})\rangle}{\delta\nu^2}. \qquad (5)$$

We observe that F is isotropic, and apart from a small peak around $R = d$, decreases approximately exponentially with R (Fig.3(a)) : $F(R) \simeq \exp(-R/L_c)$. The correlation length L_c remains smaller than the size of a grain for small cohesion, and then suddenly increases for $\eta \geq 1$ (Fig.3 (b)).



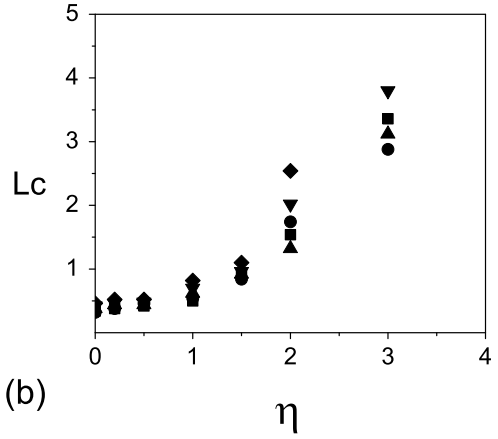


FIG. 3. Spatial heterogeneity : (a) Correlation function (η = 0; 0.5 (black line ; 1($\triangleleft$) ; 1.5($\circ$) ; 2 ($\square$) ; 3 ($\triangleright$)), (b) Length scale (I= 0.025 ($\bullet$) ;0.05 ($\blacktriangle$) ;0.1 ($\blacksquare$) ; 0.2 ($\blacktriangledown$) ; 0.3 ($\blacklozenge$)).

4.2 Persistence of contact

Starting from a population of contacts at time t, we define the function $P(T)$ as the proportion of contacts that are still active at time $t+T$ (even if they may have been broken in the meanwhile). This is similar to the so-called topological correlation function defined in ref. Choi, Kudrolli, Rosales, and Bazant (2004) to measure the diffusion in granular flows. This function should decrease from unity to zero with time T. The characteristic time of this decrease defines a persistence time T_p of the contacts. For cohesionless grains, we predict that T_p should be of the order of the shear time $1/\dot{\gamma}$ in the quasi-static regime and should decrease to the collision time in the dynamic regime. Consequently, in the dense flow regime, the average strain $D = \dot{\gamma}T$ should be more relevant than the time T. Indeed, we have observed that the curves measured for various inertial numbers collapse when drawn as a function of the average deformation D.

We observe that P decreases approximately exponentially with D (Fig.4(a)) : $P(D) \simeq \exp(-D/D_p)$. For cohesionless grains in the dense regime, D_p is of the order 1 (Fig.4(b)). Then D_p strongly increases with the intensity of the cohesion η. This indicates that the average lifetime of the clusters becomes larger than the shear time. This is consistent with the observation of the fracturation of the granular material for strong cohesion.

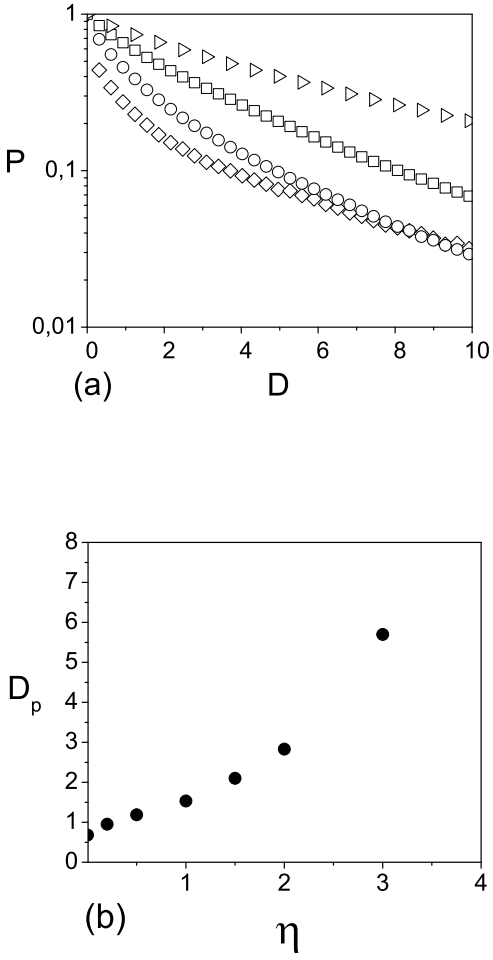


FIG. 4. Persistance of contact. (a) $P(D)$ η = 0 ($\diamond$) ; 1($\triangleleft$) ; 2($\square$) ; 3 ($\triangleright$). (b) $D_p(\eta)$.

5 CONCLUSION

Considering homogeneous steady shear flows and a simple cohesion model, we have measured the influence of cohesion on the rheology of granular materials. A viscoplastic constitutive law is deduced from the dilatancy and the friction law. As the cohesion increases, the grains agglomerates in transient clusters, which leads to a progressive expansion of the material. The analysis of the space and time correlations shows a structural transition above a crtical cohesion threshold, associated to a sudden increasze of the macroscopic friction. The quantitative understanding of the relation between the microsstructure and the rheological law remains an open question.

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