

Behavior of model cohesive grains in the dense flow regime

Pierre Rognon^{1,2}, François Chevoir^{1,†}, Mohamed Naaïm² & Jean-Noël Roux¹

¹ LMSGC, Institut Navier, 2 allée Kepler, 77 420 Champs sur Marne, France

² CEMAGREF, 2 rue de la Papeterie, BP 76, 38402 Saint-Martin d'Hères, France

† chevoir@lcpc.fr

Résumé :

Nous étudions par dynamique moléculaire la loi de comportement d'écoulements denses de grains cohésifs, en considérant un modèle de cohésion simple et générique qui rend compte de résistance maximale à la traction des contacts. La géométrie du cisaillement homogène met en évidence une dépendance simple du frottement effectif en fonction de l'état de cisaillement et de l'intensité de la cohésion. Ces variables se résument en deux nombres sans dimension, le nombre d'inertie, qui compare l'inertie des grains à la force de confinement, et le nombre de cohésion, qui compare les forces attractives à ces même forces de confinement. Dans le cas d'un écoulement sur pente, l'augmentation du frottement avec la cohésion, d'autant plus sensible près de la surface libre, provoque la formation d'un écoulement bouchon.

Abstract :

Using molecular dynamics simulations, we study the constitutive law of dense flows of cohesive grains. We focus on a simple cohesive model that takes into account the maximal attractive force between grains. The study of plane shear flows highlights a simple dependence of friction on both shear state and cohesion intensity. These two parameters are described by two dimensionless numbers, respectively the inertial number which compares the inertia of grains with the prescribed confinement force, and the cohesion number which compares attractive force with the prescribed confinement force. In the case of flow down a slope, this cohesion enhanced friction leads to plugged flow since cohesion intensity increases near the free surface.

Key-words :

Flow ; Granular ; Cohesion

1 Introduction

Dense flows of cohesionless grains have a rich rheological behavior highlighted by several studies motivated by fundamental issues as well as practical needs (see for example the review of Gdr Midi, 2004). However, granular materials outside of laboratory often present significant inter-particle cohesive forces resulting from different physical origins : *van der Waals forces* for small enough grains such as clay, powders (Rietema, 1991) or third body in tribology (Iordanoff *et al.*, 2002), *capillary forces* in humid grains such as unsaturated soils or wet snow, and *solid bridges* in sintered powders or when liquid menisci freeze. How does a cohesive force affect dense granular flows ? Up to now, this question is largely ignored. Here we present a numerical study of dense flows of a model cohesive granular material which takes into account the common feature of any cohesive grains : the maximum attractive force of contacts. In section § 2, simulated systems are described and the dimensionless numbers which control them are identified. Homogeneous plane shear flows give a direct access to the constitutive law as function of cohesion intensity, which validity is then checked for flows down inclined, closer to practical needs but more complex since stresses vary along depth (§ 3).

2 Simulated systems

The standard molecular dynamics using here is a very common method to simulate flows of grains (da Cruz *et al.*, 2005; Brewster *et al.*, 2005; Aarons and Sundaresan, 2006). It ensures to easily control and vary the parameters that describe grains, and gives access to properties within the flows. However, computational times limits the number of grains per flow to thousands. Here, low numbers of grains are considered so that several flows can be performed, allowing to explore a large range of parameters. To keep large enough simulated cells, systems are two dimensional.

The granular material is an assembly of n disks of mass m and of diameter $d \pm 20\%$. This uniform polydispersity prevails crystallization. Grains interact merely through direct contact, without long range forces neither interstitial fluid effect. The normal contact force N between two grains is split into three components which are expressed as function of the normal deflection or apparent interpenetration h , and the normal relative velocity \dot{h} :

$$N(h) = k_n h + \zeta \dot{h} - \sqrt{4k_n N^c h}. \quad (1)$$

The visco-elastic repulsion introduces the normal stiffness k_n related to the Young modulus E of grains ($k_n \sim Ed$), and a damping parameter ζ which leads to energy dissipation. Considering a binary collision between two similar grains, ζ is related to the Newton restitution coefficient e : $\zeta = \sqrt{2mk_n}(-2 \ln e)/\sqrt{\pi^2 + \ln^2 e}$. Models of cohesive interactions due to van der Waals forces (Desjardin *et al.*, 1975; Johnson *et al.*, 1971), capillary forces (Bocquet *et al.*, 2002) or solid bridges generally add to the repulsive force an attractive force $N^a(h)$ which precise form represents the physical origin of the interaction, sometimes involving long range forces and/or hysteresis. The simple forme adopted here, $N^a(h) = -\sqrt{4k_n N^c h}$, does not describe one of the three previous interactions, but merely represent their common feature giving rise to a maximal attractive force N^c for the contacts. Furthermore, grains are frictional. As usual, the tangential contact force T is described by a Coulomb condition enforced with the sole elastic part of the normal force, $|T| \leq \mu k_n h$, with μ the friction coefficient between grains, so that friction is non null total normal force is null. T is related to the relative tangential displacement δ : $T = k_t \delta$, with a tangential stiffness coefficient k_t . There is not rolling friction.

Two flow geometries are studied : the plane shear without gravity, and the rough inclined plane (see figures 1). In both cases the flows are simulated in a cell of length L and height H using periodic boundary conditions along the flow direction (x). Plane shear flows are performed prescribing both pressure P and shear rate $\dot{\gamma}$ through Lees-Edwards boundary conditions along the transverse direction y . The top and bottom cells move with a velocity $\pm V(t)$, which is adapted at each time step t to maintain a constant shear rate $\dot{\gamma} = V(t)/H(t)$. The control of the pressure is achieved by allowing the dilatancy of the shear cell along y : $\dot{H} = (P - P_0)L/g_p$, where g_p is a viscous damping parameter, and P_0 is the average pressure in the shear cell. Steady state corresponds to $\langle P_0 \rangle = P$. Flows down rough inclined are driven by gravity \vec{g} . Grains constitute a layer of thickness H flowing along a rough inclined wall (slope θ), made of contiguous grains sharing the characteristics of the flowing grains : same polydispersity and mechanical properties (especially same cohesion), but without rotation.

Both grains and flow geometries are described by a list of independent dimensional parameters. It is convenient to use dimensional analysis to extract dimensionless numbers which express the relative importance of different physical phenomena and enable quantitative comparison with real materials. Grains are described by d , m , e , μ , k_n , k_t and N^c . d and m respectively constitute the length and mass scales. The values of e , μ and k_t/k_n does not significantly affect the propeties of dense cohesionless ganular flows, as soon as $e \neq 0$, $e \neq 1$,

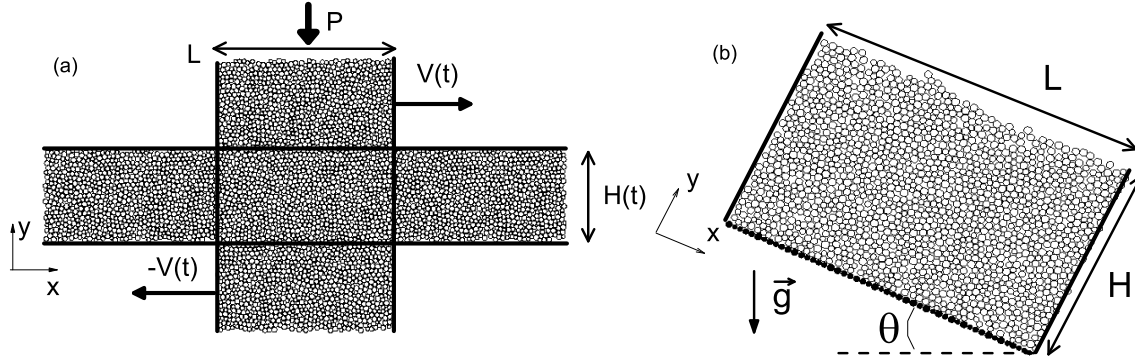


Figure 1: Flow geometries : (a) plane shear and (b) rough inclined plane. Rough walls (black grains), (—) periodic boundary conditions.

$\mu \neq 0$ and $k_t \sim k_n$ (Silbert *et al.*, 2001; da Cruz *et al.*, 2005). Consequently, we fix the fairly realistic values $k_t/k_n = 0.5$ and $\mu = 0.4$, and $e = 0.1$ which corresponds to a rather dissipative material but favors convergence toward steady states. The flows down inclined plane involves the gravity \vec{g} , the slope θ and the thickness H of the flowing layer, whilst the plane shear is described by the prescribed pressure P , the prescribed shear rate $\dot{\gamma}$, and the viscous damping parameter g_p . The dimensionless number $g_p/\sqrt{mk_n} = 1$ is chosen, so the time scale of the fluctuations of H is imposed by the material. da Cruz *et al.* (2005) have shown that shear rate of cohesionless grains is controlled by the sole *inertial number* I :

$$I = \dot{\gamma} \sqrt{\frac{m}{P}}, \quad (2)$$

which compares the inertial time $\sqrt{m/P}$ with the shear time $1/\dot{\gamma}$. A small inertial number ($I \lesssim 10^{-3}$) corresponds to the *quasi-static* regime where the grain inertia is not relevant. Inversely, a large value ($I \gtrsim 0.3$) corresponds to the *collisional* regime where grains interact through binary collisions. In between these extremes, we focus on the *dense regime* ($10^{-2} \lesssim I \lesssim 0.3$) for which grain inertia is important within a contact network percolating through particles. Cohesion intensity is usually measure by the Granular Bond Number Bo_g (Nase *et al.*, 2001) which compares the maximum attractive force with the grain weight : $Bo_g = N^c/mg$. For plane shear flows without gravity, we define a second dimensionless number η which compares N^c with the average normal force Pd due to the pressure :

$$\eta = \frac{N^c}{Pd}. \quad (3)$$

3 Constitutive law

Plane shear without gravity leads to homogeneous shear state where the effective friction coefficient $\mu^* = \tau/P$ (ratio of tangential and normal stresses), I and η are constant over space and time. For each cohesion intensity η , different shear states I are prescribed and μ^* is measured (Figure 2 a). It appears that the constitutive law of cohesionless grains (da Cruz *et al.*, 2005), i.e. a linear increases of $\mu^*(I)$ (see $\eta = 0$ on figure 2 (a)), can be generalized to cohesive grains, but with the parameters μ_s^* and b strongly enhanced by cohesion (figure 2 b) :

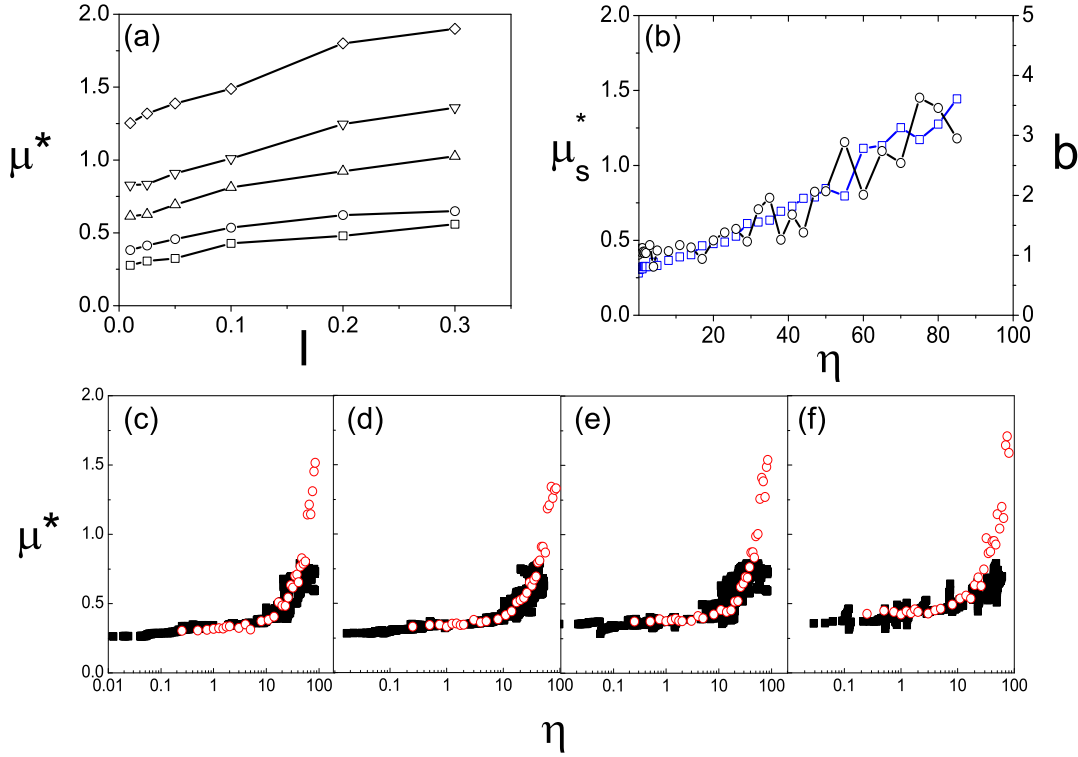


Figure 2: *Constitutive law of cohesive grains. Plane shear flow* : (a) $\mu^*(I)$ for different values of cohesion intensity $\eta = 0$ (\square), 10 (\circ), 30 (\triangle), 50 (∇), 70 (\diamond); (b) $\mu_s^*(\eta)$ (\square) and $b(\eta)$ (\circ); *comparison between measurements from homogeneous plane shear flows and flows down inclined* : $\mu^*(\eta)$ for $I = 0.01$ (c), 0.025 (d), 0.05 (e), 0.1 (f).

$$\mu^*(I, \eta) \simeq \mu_s^*(\eta) + b(\eta)I. \quad (4)$$

Let us now consider the flow down a slope θ of a layer $H \approx 30d$ of cohesive grains, for various cohesion intensity Bo_g between 0 and 200 and various slope. Without cohesion, such a flow reach a steady and uniform regime in a large range of slope, accelerate for higher slope and stop below a non null critical slope. These regimes still exists for cohesive grains, although critical slope strongly increases. For steady and uniform regime, friction exactly offsets the gravity driven force, and the solid fraction remain constant along the depth, so that stresses follow an hydrostatic profile : $[P(y), \tau(y)] \propto g(H - y) [\cos \theta, \sin \theta]$ (Gdr Midi , 2004; da Cruz *et al.*, 2005). Thus, grains within such a flow are submitted to a shear with $\mu^* = \tan \theta$ prescribed by the slope, and constant along depth. Furthermore, since the pressure increases along the depth, the cohesion number η increases when approaching to the free surface, $\eta(y) \propto Bo_g d / ((H - y))$.

Then the local constitutive law of the material can be deduced through the measurement of $I(y)$ and $\eta(y)$ for various slope, i.e. various μ^* . To reach this aim, steady and uniform flows are initially performed at a given slope for various Bo_g , then slope is decreased (or increased) at a low enough rate so that flows can be considered as steady and uniform at each time step, until the

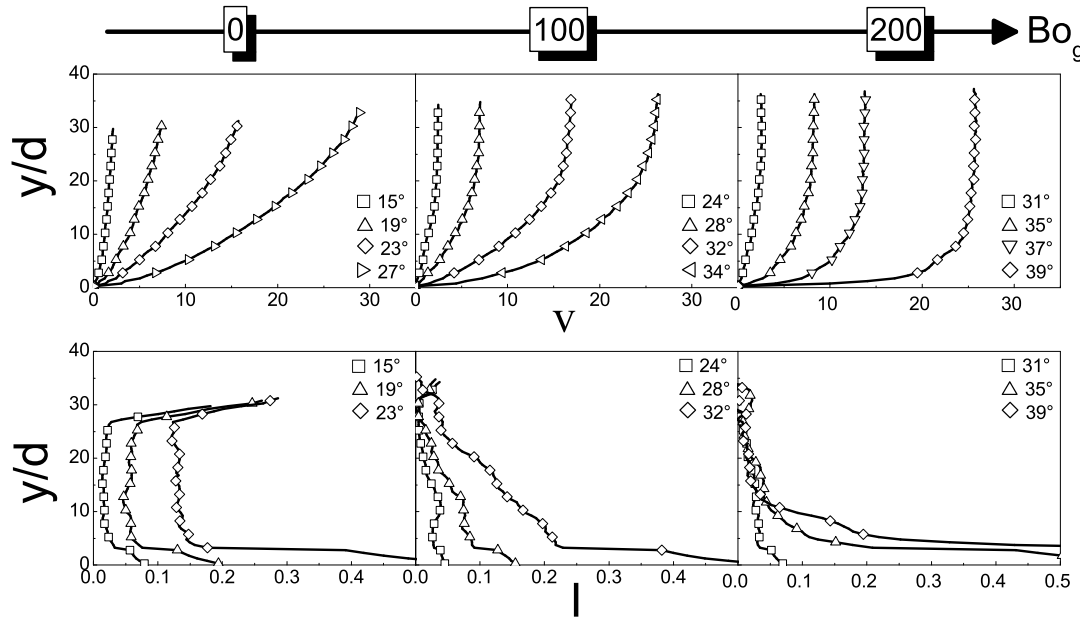


Figure 3: Steady and uniform cohesive flow down inclined : velocity profile $v(y)$ (in \sqrt{gd} units) and inertial number profile $I(y)$ for various Granular Bond Number Bo_g , and various slope θ (details on graphics).

flows stop (or until the flow accelerated). The figures 3 plot the velocity profile and the profile of inertial number for various slope and various Bo_g . Without cohesion ($Bo_g = 0$), velocity profiles follow the Bagnold scaling $\dot{\gamma}(y) \propto (H - y)$, since the inertial number is constant along the depth, excepted for the first bottom layers where I increases due to the proximity of the wall, and the first free surface layers where I diverges due to the low pressure (da Cruz *et al.*, 2005; Gdr Midi, 2004). With cohesive force, there appears a plugged layer at the free surface where the shear rate drop to zero. The thickness of this layer increases as Bo_g increases. This breakdown of the Bagnold scaling, observed by Brewster *et al.* (2005), is evidenced by the inertial number which is no more constant along depth, and drops to zero in the plugged surface layer.

Figures 2(c-f) plot $\mu^*(\eta)$ for various I , and compare the results obtained using inclined plane with the constitutive law measured using plane shear flows. Results are in good agreement, although data from inclined plane are scattered. This is not surprising since they are not averaged over time, neither over transverse direction. The great difference between these two geometries is that the shear rate is prescribed in plane shear whereas shear stress is prescribed in flows down inclined plane. As a consequence, large value of I and strong cohesion, which can be explored using plane shear cannot be reached within flow down inclined since the most cohesive part of the flow is plugged.

4 Conclusions

This numerical study provides new insights about dense flows of cohesive grains. First, homogeneous plane shear flows have been performed, prescribing various values of two dimension-

less number which control the shear state (inertial number) and the cohesion intensity (cohesion number). This method gives a direct access to the constitutive law of cohesive grains, which can be expressed in a simple form similar to the one of cohesionless grains : the effective friction coefficient still linearly increases with the inertial number but is strongly enhanced as cohesion intensity increases. Then, the consequence of such a behavior have been pointed out in the case of cohesive flows down a slope. As soon as the cohesion intensity increases when approaching to the free surface, the shear rate drop to zero in this area which leads to plugged flows. The comparison between constitutive law measured within homogeneous plane shear flows and within flows down inclined reveals a good agreement. Nevertheless, the bottom layers are affected by the roughness so that they cannot be described by the sole constitutive law.

The reference Rognon *et al.* (2005) gives more details about plane shear of cohesive grains, focusing on the strong interplay between constitutive law and the properties at the scale of the grains and of the contact network.

References

- L. Aarons and S. Sundaresan. Shear flow of assemblies of cohesive and non-cohesive granular materials. *Powder Tech.*, 169:10–20, 2006.
- L. Bocquet, E. Charlaix, and F. Restagno. Physics of humid granular media. *Compte Rendu Physique*, 3:207–215, 2002.
- R. Brewster, G.S. Grest, J.W. Landry, and A.J. Levine. Plug flow and the breakdown of Bagnold scaling in cohesive granular flows. *Phys. Rev. E*, 72:061301, 2005.
- F. da Cruz, S. Emam, M. Prochnow, J-N. Roux, and F. Chevoir. Rheophysics of dense granular materials : Discrete simulation of plane shear flows. *Phys. Rev. E*, 72:021309, 2005.
- B.V. Derjaguin, V.M. Muller, and Y.P. Toporov. Effect of contact deformation on the adhesion of particules. *J. Coll. Inter. Sci.*, 53:314–326, 1975.
- GdR MiDi. On dense granular flows. *Euro. Phys. J. E*, 14:341–365, 2004.
- I. Iordanoff, B. Sève, and Y. Berthier. Solid third body analysis using a discrete approach : influence of adhesion and particle size on the macroscopic behavior of the contact. *J. Tribology*, 124:530–538, 2002.
- K. L. Johnson, K. Kendall, and A.D. Roberts. Surface energy and contact of elastic solids. *Proc. Roy. Acad. London A*, 324:301–324, 1971.
- S.T. Nase, W.L. Vargas, A. Abatan, and J.J. McCarthy. Discrete characterization tools for cohesive granular material. *Powder Tech.*, 116:214–223, 2001.
- K. Rietema. *The dynamics of fine powders*. Elsevier, New York, 1991.
- P. G. Rognon, J-N. Roux, D. Wolf, M. Naaim, and F. Chevoir. Rheophysics of cohesive granular materials. 74:644–650, 2006.
- S. L. Silbert, D. Ertas, G. S. Grest, T.C. Halsey, D. Levine, and S. J. Plimpton. Granular flow down an inclined plane. *Phys. Rev. E*, 64:385–403, 2001.