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Behavior of model cohesive granular materials in the dense flow regime

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Résumé :

La simulation numérique discrète (dynamique moléculaire) est appliquée à la détermination d'un loi de comportement pour les écoulements denses de grains cohésifs. Nous utilisons un modèle de contact simple et générique dont les paramètres essentiels sont la traction maximale dans un contact et le coefficient de frottement intergranulaire. La géométrie du cisaillement homogène met en évidence une dépendance simple du frottement interne 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 et le nombre de cohésion, qui comparent respectivement l'inertie des grains et les forces attractives à la force de confinement. Dans le cas d'un écoulement gravitaire sur une pente, l'augmentation du frottement près de la surface libre, où le nombre de cohésion est maximal, entraîne la formation d'un écoulement bouchon.

Abstract :

Molecular dynamics simulations are applied to the study of the constitutive law for dense flows of cohesive grains. We focus on a simple cohesive model in which the important parameters are the tensile strength and the friction coefficient in contacts. The study of plane shear flows highlights a simple dependence of the macroscopic internal friction law on both the shear state and the cohesion intensity. Such state variables boil down to two dimensionless parameters, the inertial number and the cohesion number, which respectively compare the inertia of grains and the attractive forces with the applied confining forces. In the case of a gravity-driven flow down a slope, the cohesion number increases near the free surface, where cohesion-enhanced friction leads to plug flow.

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 by Gdr Midi, 2004). However, granular materials outside the laboratory often present significant interparticle cohesive forces due to different physical origins : *van der Waals forces* for small enough grains, as in clays and powders Rietema (1991) or within the third body in tribology Jordanoff *et al.* (2002), *capillary forces* between the humid grains of unsaturated soils or wet snow, and *solid bridges* in sintered powders or when liquid menisci freeze. The possible influence of cohesive forces on dense granular flows has been largely ignored so far. The present numerical study addresses this issue with a model cohesive granular material, in which the tensile strength of intergranular contacts – a common feature of cohesive granular materials – plays a central role. Section 2 describes the simulated systems and defines the dimensionless numbers, which are used as control parameters. Homogeneous plane shear flows, as studied in Sec. 3, give a direct access to the constitutive law involving the cohesion number. Its validity is then checked for flows down inclines, and we end with a brief conclusion (Sec. 4).

2 Simulated systems

The standard implementation of molecular dynamics we are using here is commonly applied to granular flows da Cruz *et al.* (2005); Brewster *et al.* (2005); Aarons and Sundaresan (2006). Discrete simulations enable detailed studies of the influence of micromechanical parameters and of the inner state of flowing granulates. However, computational times restricts the number of grains to thousands. Here we use a two-dimensional model and our numerical samples have a relatively small number of grains. This allows us to explore a large range of parameters.

The granular material is an assembly of n disks of mass m and of diameter $d \pm 20\%$. This uniform polydispersity avoids crystallization. Grains interact merely through direct contact, without distant attractive forces, or interstitial fluid effect. The normal contact force N between two grains is split into three components which are expressed as functions of the normal deflection or apparent interpenetration h , and the normal relative velocity \dot{h} :

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

Eqn. 1 involves a normal stiffness k_n related to the Young modulus E of the grains ($k_n \sim Ed$), and a damping parameter ζ which leads to energy dissipation. Considering a binary head-on collision between two similar grains devoid of cohesion, 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 Derjaguin *et al.* (1975); Johnson *et al.* (1971), capillary forces Bocquet *et al.* (2002) or solid bridges generally add to those repulsive contributions an attractive term $N^a(h)$, the specific form of which depends on the physical origin of the interaction, sometimes involving long range forces and/or hysteresis. The simple form adopted here, $N^a(h) = -\sqrt{4k_n N^c h}$, does not accurately describe any one of those interactions, but accounts for one essential common feature, the pull-off force N^c (maximum attraction) in the contacts.

Furthermore, grains are frictional. 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. Note that a contact in which the total normal force is zero might carry a nonvanishing tangential force. T is related to the relative *elastic* tangential displacement δ : $T = k_t \delta$, with a tangential stiffness coefficient k_t . There is not rolling friction.

Two flow geometries are studied: plane shear without gravity, and the rough inclined plane (see Figs. 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 studied on prescribing both the pressure, P and the shear rate, $\dot{\gamma}$, through Lees-Edwards boundary conditions. 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 for some 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 $\langle P \rangle = P_0$. Flows down rough inclines are driven by gravity \vec{g} . A granular layer of thickness H flows down a rough inclined plane (slope θ), which is made of a rigidly assembled row of fixed, contacting grains with the same geometric characteristics and contact parameters as the flowing ones.

It is convenient to use dimensional analysis, as the resulting dimensionless numbers 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 set the length and mass units. The values of e , μ and k_t/k_n do not significantly affect the properties of dense cohesionless granular flows, as soon as $e \neq 0$, $e \neq 1$, $\mu \neq 0$ and $k_t \sim k_n$ Silbert *et al.* (2001); da Cruz *et al.* (2005). Consequently, we fix the fairly realistic values

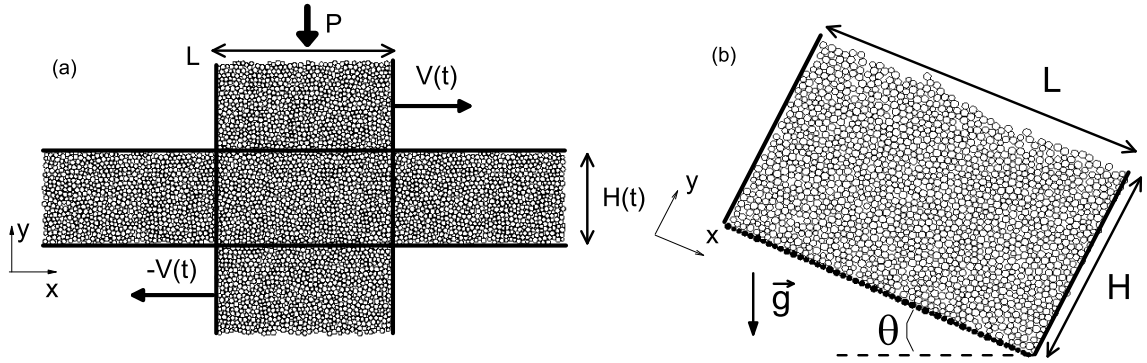


Figure 1: Flow geometries : (a) plane shear and (b) rough inclined plane. Rough walls (black grains), (—) periodic boundary conditions.

$k_t/k_n = 0.5$ and $\mu = 0.4$, and $e = 0.1$ which corresponds to a rather dissipative material but favors evolutions toward steady states. Flows down inclined planes involve gravity \vec{g} , the slope θ and the thickness H of the flowing layer, whilst plane shear is described by the applied normal 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 that the time scale of the fluctuations of H is imposed by the material. da Cruz *et al.* (2005) have shown that the state of assemblies of cohesionless grains in dense shear flows 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 shearing 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 extreme cases, 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 the particle pack. Cohesion intensity is usually measured 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 flows without gravity leads to homogeneous states where the effective friction coefficient $\mu^* = \tau/P$ (*i. e.*, the ratio of tangential to normal stresses on a surface parallel to the flow direction) as well as numbers I and η are constant over space and time. For each cohesion intensity η , different shear states I are prescribed and μ^* is measured (Fig. 2 a). It appears that the constitutive law of cohesionless grains da Cruz *et al.* (2005), *i. e.*, a linear increase of $\mu^*(I)$ (see $\eta = 0$ on figure 2 (a)), can be generalized to cohesive grains, parameters μ_s^* and b strongly

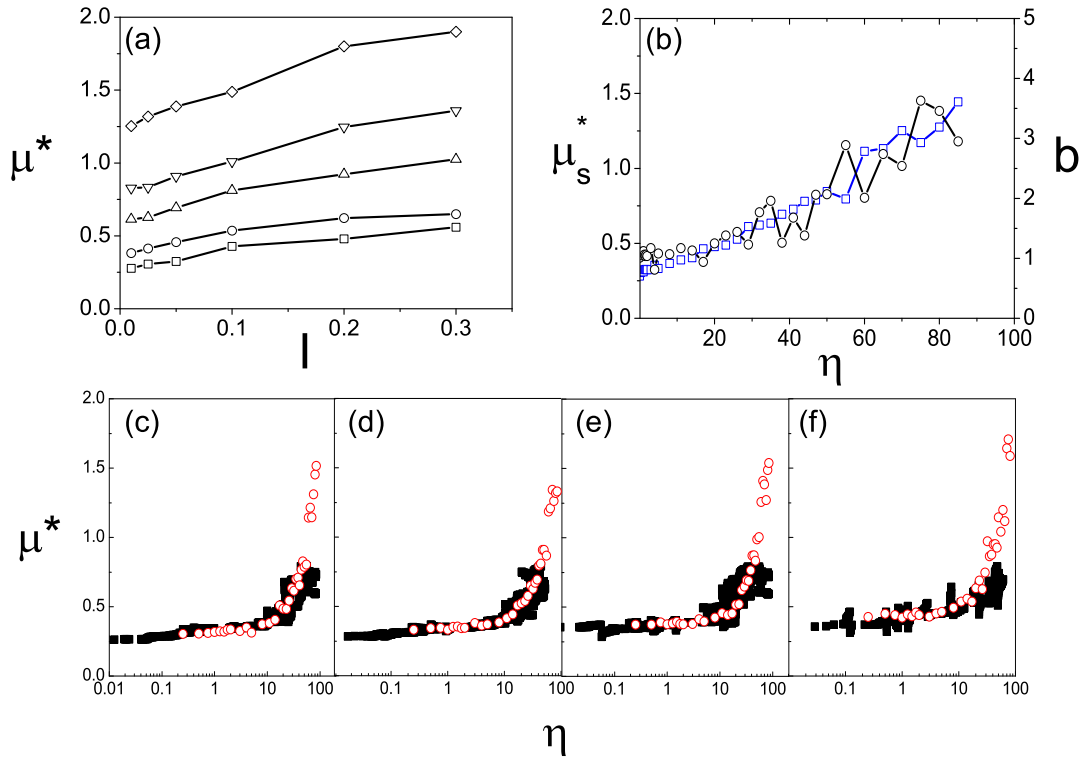


Figure 2: Constitutive law of cohesive grains. Plane shear flow : (a) $\mu^*(I)$ for different values of cohesion intensity $\eta = 0$ (\square), 10 (\circ), 30 (\triangle), 50 (∇), 70 (\diamond); (b) $\mu_s^*(\eta)$ (\square) and $b(\eta)$ (\circ); comparison between measurements in homogeneous plane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

enhanced by cohesion (Fig. 2 b) :

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

We now consider flows down slopes, forming different angles θ with the horizontal direction, of a cohesive granular layer of thickness $H \approx 30d$, for Bond numbers Bo_g between 0 and 200. Without cohesion, such flows reach a steady and uniform states over some θ interval. They are accelerated for steeper slopes and stop below some finite critical angle. These regimes still exist with cohesive grains, although stopping angles can be considerably larger. In steady uniform flows, internal friction exactly balances the weight, and the solid fraction is observed to remain roughly constant along the depth. The stress profile is therefore hydrostatic: $[P(y), \tau(y)] \propto g(H - y) [\cos \theta, \sin \theta]$ Gdr Midi (2004); da Cruz *et al.* (2005). Thus, in such a flow, the ratio of shear to normal stress in grain layers parallel to the bottom is constant, equal to an effective internal friction coefficient determined by the inclination angle: $\mu^* = \tan \theta$. The cohesion number η increases on approaching the free surface, $\eta(y) \propto Bo_g d / (H - y)$.

Then the local constitutive law of the material can be deduced from the measurement of $I(y)$ and $\eta(y)$ for various angles, *i.e.*, various μ^* . To this end, steady and uniform flows are initially launched at a given slope for various Bo_g , then θ is decreased (or increased) at a low

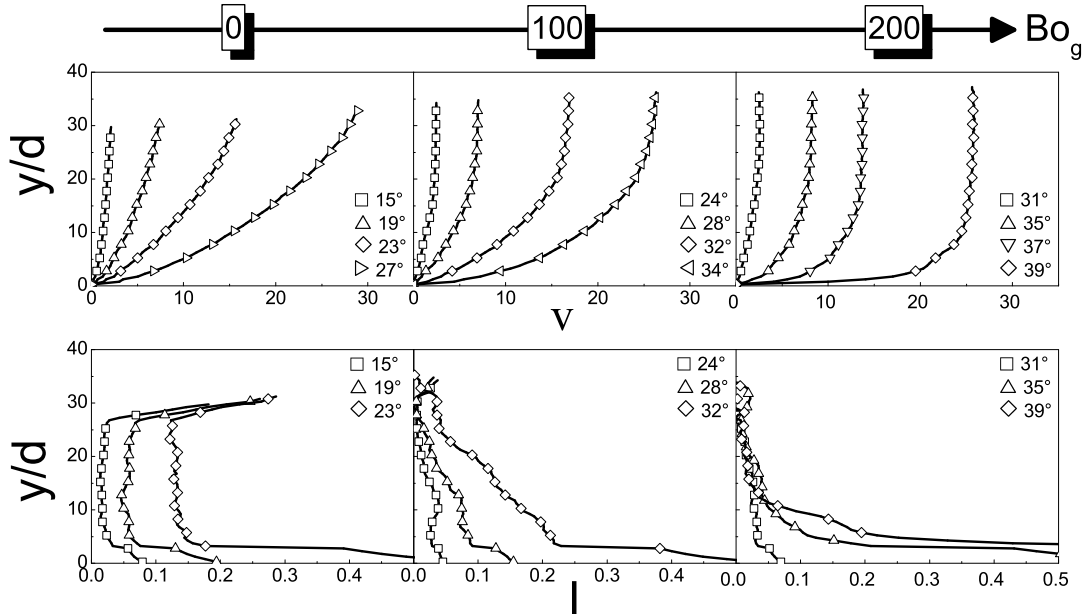


Figure 3: Steady and uniform cohesive flow down inclines: velocity profile $v(y)$ (in \sqrt{gd} units) and inertial number profile $I(y)$ for various values of granular Bond number Bo_g , and various slopes θ .

enough rate so that flows can be regarded as steady and uniform at each time step, until the flow stops (or until it accelerates). On Fig. 3 we plot the velocity and inertial number profiles for different values of θ and Bo_g . Without cohesion ($Bo_g = 0$), the velocity profiles abide by the Bagnold scaling $\dot{\gamma}(y) \propto (H - y)$, because the inertial number is constant along the depth (except 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 cohesion, plug flow develops in a layer near the free surface, where the shear rate drops to zero. The thickness of this layer increases with Bo_g . 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 plug flow layer.

Figs. 2(c-f) plot $\mu^*(\eta)$ for various I , and compare the results obtained using inclined planes with the constitutive law measured in homogeneous 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 coordinate y . The great difference between these two flow geometries is that the shear rate is prescribed in plane shear flows whereas the shear stress is prescribed in flows down inclined planes. As a consequence, large values of I and strong cohesion, which can be explored in homogeneous plane shear flows cannot be reached in the inclined plane geometry, for which the shear rate drops to zero in the high cohesion number region.

4 Conclusions

This numerical study provides new insights about dense flows of cohesive grains. First, a study of homogeneous plane shear flows, depending on inertial number I (a reduced shear rate) and

cohesion number η (a reduced cohesion intensity), enabled us to directly determine the constitutive law, in a simple form similar to the one used for cohesionless grains. The effective friction coefficient varies linearly with I , inertial number but is strongly increased for large η values. The subsequent study of cohesive flows down slopes evidenced the consequences of such a rheological behaviour, the increase of cohesion intensity leading to plug flow (vanishing strain rate) near the free surface. Despite specific boundary effects affecting the material a few grain diameters away from the rough plane, the same constitutive law consistently applies to both flow geometries.

Rognon *et al.* (2006) give more details about the inner state of model cohesive granular materials in plane shear flows of cohesive grains, focussing on the strong interplay between constitutive laws and grain-scale properties and contact networks.

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