Model cohesive powders: assembling process and plastic consolidation

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Résumé :

Nous appliquons la simulation numérique de type éléments discrets à l’étude de l’assemblage et de la consolidation plastique isotrope de poudres cohésives modélisées d’agrégats bidimensionnels de disques. L’état du matériau est fonction d’une pression réduite \( P^* \) qui compare la pression de confinement à la force attractive maximale dans les contacts, et il est très sensible au processus d’assemblage. Lorsque les grains s’agrègent et forment une structure continue avant application d’un confinement, on obtient des configurations lâches, fractales, avec la dimension des amas produits par agrégation balistique aux échelles intermédiaires entre le diamètre de la particule et une certaine taille de blob \( \xi \). La coordination varie avec le niveau d’agitation initiale et avec la résistance au roulement. Sous \( P^* \) croissante on assiste à un effondrement plastique (irréversible) analogue à la consolidation des argiles et des poudres au cours duquel la taille caractéristique \( \sim \xi \) des plus grands pores diminue et le système retrouve peu à peu la microstructure des assemblages granulaires non cohésifs.

Abstract :

Discrete element simulations are used to investigate the assembling and the plastic consolidation behavior of model cohesive powders which consist of two-dimensional aggregates of disks. The material state varies with a reduced pressure \( P^* \) comparing the confining pressure to the maximum tensile contact force, and sensitively depends on the assembling process. If in initially a continuous structure has formed before the confining stress is applied, loose configurations are obtained, with the fractal dimension of ballistic aggregation clusters characterizing density correlations on scales between the grain size and a certain blob size \( \xi \). The coordination number varies with the initial agitation velocity and with the resistance to rolling in contacts. Under growing \( P^* \), the system undergoes an irreversible collapse similar to the plastic consolidation of clays and powders in which the characteristic size \( \sim \xi \) of the larger pores decreases and the microstructure of cohesionless granular assemblies is gradually recovered.

Keywords: cohesion ; granular materials ; powders

1 Introduction

Unlike cohesionless granular packings, which are chiefly sensitive to stress direction, rather than intensity, cohesive systems like clays (Mitchell 1993) or powders (Castellanos 2005) undergo significant porosity reductions along proportionally growing stress paths. Assemblies of rotund-shaped particles can be stable with packing fractions \( \Phi \) as low as 20% (Castellanos 2005), and their tenuous structure collapse as they get much more closely packed on increasing the confining pressure. Such a behaviour is studied here with DEM simulations of a model 2D material, presented in Sec. 2. Its geometry, and some micromechanical aspects are studied and shown to sensitively depend on the assembling process in Sec. 3. We then report on plastic collapse under growing load (Sec. 4), and end up with a few conclusive remarks (Sec. 5). More details can be found in recent papers (Gilabert et al. 2007a; Gilabert et al. 2007b).
2 Model material and relevant control parameters

We consider as a model system an assembly of \( N \) disks with uniformly distributed diameters between \( a/2 \) and \( a \), interacting via the standard spring-dashpot contact law, suitably modified to include cohesion. The normal contact force comprises an elastic part \( N_e = K_N h \), repulsive and proportional to contact deflection \( h \), supplemented with a viscous force \( \zeta \dot{h} \), opposing the relative motion, and with an attraction term \( N_a \) equal to \(-F_0\) for contacting grains, and equal to \(-F_0(1 - |h|/D_0)\) for grains separated by distance \(-h\) between 0 and \( D_0 \) (\( H \) is the Heaviside step function). The law for tangential force \( T \) is elastoplastic incremental, limited by a Coulomb inequality implying the sole elastic repulsive normal force: \( |T| \leq \mu K_N h H(h) \). It involves linear elastic tangential elasticity with stiffness \( K_T \). Fig. 1 is a schematic representation of the static part of the contact law. In addition one optionnally introduces rolling resistance (RR), with the model proposed by Tordesillas & Stuart (2002) for the local rolling moments \( \Gamma \) at contact points. \( \Gamma \) opposes the relative rotation of the grains. Its value is limited by a rolling friction coefficient \( \mu_r \), which is related to the asperity scale on the grain surfaces, so that \( |\Gamma| \leq \mu_r N_e \). An external pressure \( P \) is applied on manipulating the periodic boundary conditions for rectangular cells, as suggested by Parrinello & Rahman (1981). On externally increasing stresses \( \sigma_{11} = \sigma_{22} = P \), the simulation shrinks until forces and torques balance on each grain, while, for \( \alpha = 1, 2 \),

\[
\sigma_{\alpha \alpha} = \frac{1}{2A} \sum_{i=1}^{N} \sum_{j \neq i} N_{ij}^{(\alpha)} r_{ij}^{(\alpha)},
\]

in which \( A \) is the 2D sample area, and \( r_{ij} \) the branch vector from the centre of disk \( i \) to that of disk \( j \) expresses global static stress balance (Christoffersen et al. 1981).

It is important (Gilabert et al. 2007a) to note that contacts may carry tangential forces (as large as \( \mu F_0 \)) and, with RR, rolling moments (as large as \( \mu_r F_0 \)) while the total normal force is equal to zero, as in an isolated contacting pair, due to the compensation of elastic repulsion and adhesive force \( F_0 \), \( N_e + N_a = 0 \).

Most calculations were done with the following parameters:

\[
K_N = K_T = 10^5 \frac{F_0}{a}; \quad \mu = 0.5; \quad \mu_r = 0.01a \text{ or } \mu_r = 0; \quad \frac{D_0}{a} = 10^{-3}
\]
We focus in the sequel on systems with RR, as we observed that even a small value of $\mu_r$ qualitatively changes the results, and because some small RR is necessarily present in practice, due to particle shape irregularities.

An important dimensionless quantity is the reduced pressure $P^* = aP/F_0$, expressing the competition between adhesive and confining forces. Under low $P^*$ cohesion dominates, positive (repulsive) and negative contact forces have to compensate. Under high $P^*$ the external confining load dominates, and the effects of cohesive forces should become negligible.

The high contact stiffnesses chosen correspond to the appropriate range for ratio $K_N a/F_0$ in the cohesive xerographic toner particles described by Castellanos (2005), and ensure that contact deflections have negligible geometric effects even under high $P^*$ when the confining load dominates adhesive forces.

3 Assembling process and low consolidation states

If a low pressure is applied to a cloud of initially immobile isolated grains until one single aggregate stabilizes, one obtains rather dense configurations, with $\Phi$ above 70% with our choice of parameters. In order to produce loose samples, on which we focus in the sequel, it is necessary to initially set the grains into motion, with random velocities, the mean quadratic value being denoted as $V_0$, and let them aggregate before turning on confining stresses. $V_0$ should be compared to the velocity $\sqrt{D_0 F_0/m}$ necessary to escape the potential energy of attraction (See Fig. 3a below), most calculations being done with a somewhat intermediate value in this respect. Typical aspects of equilibrated configurations with RR under zero pressure are shown on Fig. 2. Only hyperstatic structures, which with RR simply means those possessing contact loops, can carry non-zero forces. For such loops to close, since one contact can stabilize a grain
with RR, it is necessary to break and rearrange tenuous structures, which is favoured by large $V_0$ and small $\mu_r$ values. Consequently, self-balanced contact forces appearing on Fig. 2(a), showing a configuration with small RR and $V_0 = 0.3\sqrt{D_0F_0/m}$, are virtually absent on Fig. 2(b), corresponding to nearly loopless configurations with large RR (main picture) or small $V_0$ (inset). The influence of $V_0$ on coordination number $z$ is shown on Fig. 3(a). $z$ is obviously not determined by the density alone, it is sensitive to the sample history.

When ballistic aggregates form, as in the initial preparation stage of the samples we are studying here, a fractal structure is built, characterizing density correlations on scales $\gg a$. The fractal structures resulting from ideal aggregation processes, in which the aggregates cannot break and the choice of a “sticking rule” bypasses all mechanical modelling, have been studied for decades. Refs. Smirnov (1990) and Meakin (1999) provide useful reviews. The fractal structures resulting from ideal aggregation processes, in which the aggregates cannot break and the choice of a “sticking rule” bypasses all mechanical modelling, have been studied for decades. Refs. Smirnov (1990) and Meakin (1999) provide useful reviews. The fractal behaviour at intermediate scale is evidenced on Fig. 3(b) displaying structure factors $S(k)$ (i.e., Fourier transforms of density correlation functions). As a function of wavevector $k$, $S(k)$ should decrease as a power law – see (Gilabert et al. 2007a) and references therein – with exponent $-d_F$ for $a \ll \frac{\xi}{k} \ll \xi$. Fig. 3(b) exhibits such a behaviour, one identifies the value $d_F \simeq 1.55$ corresponding to the universal result of ballistic aggregation in 2D (Smirnov 1990), while $\xi$ decreases from $\sim 9.5a$ to $\sim 5a$ as $P^*$ grows from 0 to 0.01. ($d_F$ is identified from the straight part of the decreasing $S(k)$ curve on the logarithmic plot, and a value of $\xi$ is extracted either from the fit to a certain functional form given in (Gilabert et al. 2007a), or, with very similar results, from the distribution of pore sizes). It is remarkable that this value is retrieved in samples of the kind shown on Fig. 2(a), in which the fragility of tenuous clusters in the assembling stage increased the coordination number from $z = 2$ to about 2.66: the ballistic aggregation rule states that particles that stick form one solid indeformable object and leads to loopless structures with $z = 2$. It is only satisfied here for small $V_0$ and/or large enough $\mu_r$.

![Figure 3](image_url)

Figure 3: (a) Effect of $V_0$ (and $K_N$) on $z$. (b) Structure factors at 0 and low $P^*$. (b) Structure factors in samples made with the value of $V_0$ indicated by the arrow, and small RR. Continuous lines are fits to a functional form suitable for a fractal range up to a length $\xi$. 

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4 Isotropic compression behaviour

Figure 4: Solid fraction $\Phi$ (a) and coordination number $z$ (b) in pressure cycle, with (RR) and without (NRR) a small resistance to rolling in contacts. Corresponding micromechanical parameters are given in (1), initial mean quadratic velocity was $V_0 = 0.3\sqrt{F_0D_0/m}$ and initial packing fraction 0.36 at $P = 0$.

Fig. 4 shows the effects on density and coordination of a pressure cycle, from the loose state similar to the one shown Fig. 2(a) (but a larger initial density) to a dense packing similar to that of cohesionless particles. To compute those states we stepwise increase $P$ (by factors of $10^{1/8} \approx 1.33$) and wait for mechanical equilibrium. We observe an irreversible density increase, as denser states remain stable upon decompressing. While density increases, $\xi$ decreases, at constant fractal dimension $d_F$, until a fractal range can no longer be identified. The scaling $\xi \propto \Phi^{-1/(d_F-d)}$ is roughly satisfied.

The curve can be roughly described with a straight line if expressed as the solid fraction $\Phi$ (or void index) versus $\log P$, which is familiar in soil mechanics (Mitchell 1993). The dependence of $\Phi$ on pressure, which is similar to the “consolidation curve” of cohesive soils, also resembles the behaviour of the xerographic toners studied in the Seville group (Castellanos 2005). With those materials, the contact behaviour is fairly well known: with $a \sim 10\mu m$, $F_0$ is a a few tens of nN, and irreversible compaction is the fastest for $P \sim 100$ Pa, corresponding to a value of the (3D) reduced pressure $P^* = P/(F_0a^2) \sim 1$.

Additional results (Gilabert, Roux, & Castellanos 2007b) (not presented here) show that such a curve is steeper with more fragile initial states. All other things staying equal, the irreversible collapse of loose configurations under growing $P$ is faster for poorly connected initial structures.

5 Conclusions

Let us summarize the main results.

- The reduced pressure $P^*$ is the most relevant dimensionless parameter which determines the stability of loose states and the plastic compaction behaviour.

- Loose states are obtained if some initial agitation creates large clusters before the confinement forces take over.

- There is no general relationship between density and coordination number.
• The fractal dimension of loose structures appears to be the same as the one obtained in ideal, purely geometric aggregation models (e.g., ballistic aggregation).

• However, the coordination number varies according to the ability of the initial agitation to break tenuous structures.

• The plastic consolidation curve has the same typical shape $\Delta \Phi \propto \Delta \log P$ as in experiments on different materials, although the possible effects of plastic behaviour at the level of one contact have not been included in the numerical model.

• This curve is sensitive to the initial level of agitation as well as to the rolling resistance parameters in contacts.

Clearly, the mechanical behaviour of cohesive granular assemblies, which may be equilibrated in a much larger variety of geometric configurations than cohesionless ones, remains largely unexplored and many more numerical studies are necessary (on 3D systems in particular), as well as detailed experiments providing mechanical information at the contact level.

References


