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Numerical modeling of granular material fragmentation by using Discrete Element Method

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Abstract. The aim of this study is the modeling of the fragmentation of granular material subjected to compressive loading by using *Discrete Element Method (DEM)*. The proposed model depends mainly on two mechanical aspects which are: the mechanical behavior of the granular material and the yield strength predicting the fragmentation of grains. In order to better understand the mechanical phenomena, we have studied the contact force chains according to the granulometry of the material and the fragmentation modes of grains. The proposed modeling has been tested on a numerical simulation of oedometric test by using our software *MULTICOR*.

Keywords: granular material, DEM, fragmentation, strength criteria.

1 Introduction

The crushing (or grinding) process is usually used in many industrial fields such as: pharmaceutical, mineral or food. It is well known that this process remains economically expensive, essentially due to the energetic cost and the low quality of finished products (heterogeneity of grain size and shape). In fact, the economic stakes are large as for the optimization of such process. Two solutions are commonly proposed to cure these problems: the first solution is based on the technological aspects while the second one is based on physical aspects. As regards the technological solutions, they are mainly based on the choice of the engine type to be used in order to obtain a powerful installation of crushing process and which could be adapted for granular material. However, these technological optimizations haven't given satisfactory results because the production cost remains so much expensive. In fact, it seems to be important to take into account physical aspects in order to better understand the mechanical phenomena during the process. Few years ago, many authors have suggested predictive models about physical parameters (friction and wear coefficients). Generally, these models are based on approaches of chemical engineering, but they are not appropriated to study the force chains distribution into the granular material and the prediction of fragmentation process of grains.

Our goal, through out this study, consists to develop a discrete model for granular material behavior subjected to compressive stresses by using *DEM* (Aström and Herrmann, 1998),

(Morris *et al.* 1998) and (Morikawa, 1998). This modeling depends on two mechanical aspects which are: the mechanical behavior of the granular material and the yield strength for the prediction of grain fragmentation. In order to better understand the mechanical phenomena, we must answer the following questions:

- How the contact forces are distributed into the granular material subjected to compressive stresses and how the contact forces are organized according to the granulometry of the material?
- Which mechanisms are brought into play in the fragmentation of grains and which impact the granulometry have on the fragmentation modes?
- Which overall behavior for the granular media during the process of crushing and which contribution of each particle during the process of fragmentation?

2 Mechanical approach with DEM

The conventional *DEM* allows to model really deformable particles as well as complex shapes (from the ellipsoid to the polygon). Here, we have studied the simple case of non-deformable and non penetrable particles in 2D with the computational software MULTICOR, developed by Fortin *et al.* (2004). The coordinates and the rotations of Euler are the configuration parameters q. The gyroscopic and centrifugal terms are equal to zero in 2D. The matrix of generalized mass M of the system doesn't depend on q that is diagonal block. The mechanical equation (1) can be written in the following form:

$$M \ddot{q} = F_{ext}(q, \dot{q}, t) + R^{\alpha}$$
(1)

where F_{ext} represents the known external forces and R^{α} the unknown interior forces related to contact reactions and α the contact number.

In a system composed of p heterogeneous particles (Figure 1), the critical parameter for the modeling time is the maximum number of interactions between particles. The more the interaction range is important the more we have to test the possible interactions between particles. MULTICOR uses the partitioning method coupled to a connectivity table (Fortin and Coorevits, 2003). This technique allows to reduce considerably the computational time. In that case, the computational time no longer increases like $O(p^2)$ but only like O(p), which is almost optimal. For each couple of particles Ω_i and Ω_j which may enter in contact, is associated with a local reference whose axes are oriented according to the two unit vectors n and t, respectively normal and tangential vectors in the contact plan. The normal n is directed from Ω_i and Ω_j . The variables put in duality are u^{ij} , the relative local velocity of Ω_i compared to Ω_j , and the contact reaction r^{ij} of Ω_i and Ω_j . In the local base, they are written by equations (2):

$$\dot{u}^{ij} = \dot{u}_t^{ij} + \dot{u}_n^{ij}n, \qquad r^{ij} = r_t^{ij} + r_n^{ij}n \tag{2}$$

where \dot{u}_n^{ij} is the normal separation velocity, \dot{u}_t^{ij} the sliding velocity, r_n^{ij} the contact pressure and r_t^{ij} the adherence force.



Figure.1. Granular media and its kinematic parameters.

The introduction of Coulomb's friction μ leads to a non linear problem which can't be solved by a linear programming method. Unlike the usual approach, the bipotential method leads to a single variational principle and an inequality (Fortin *et al.* 2004). By using Usawa's algorithm, we obtain a resolution algorithm of the constitutive law based on the predictive-corrective scheme expressed by equations (3):

$$predictor: \tau^{ij} = r^{ij} - \gamma \left[\dot{u}_t^{ij} + \left(\dot{u}_n^{ij} + \mu \right\| - \dot{u}_t^{ij} \right\| \right) . n \right] ,$$

$$corrector: r^{ij} = proj \left(\tau^{ij}, K_u \right)$$
(3)

where γ is a numerical parameter and K_{μ} the Coulomb's cone.

The projection of the prediction τ^{ij} on the Coulomb's cone K_{μ} leads to one of these states: non contact, contact with adherence or sliding contact. Conventionally, at each time step, the contact forces in the system are determined repeatedly by the method of successive balances based on a Gauss-Seidel algorithm for the 2D version. Each contact force is calculated by adopting temporary values over the other contacts. The convergence is obtained when the force confirms the unilateral contact law with dry friction.

3 Mean stress tensor of granular material

In order to understand the different mechanisms governing the fragmentation of the grains subjected to compressive loading, we must be able to calculate the mean stress tensor into the granular material. The knowledge of stress field, acting in the granular material, permits to give a prediction of fragmentation of grains with respect the yield strength of the granular material. Let us consider a Representative Elementary Volume (*REV*) containing N_p grains separated by voids (Figure 2).

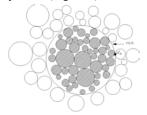


Figure.2. REV of granular material.

Modelizing grains as rigid solids in punctual contact for each grains p occupying the volume V_p , the expression of mean stress tensor is given by the following equation (4):

$$\sigma_{p} = \frac{l}{V_{p}} \left[\int_{V_{p}} q \otimes \rho \left(g - \ddot{q} \right) dV + \sum_{\alpha} q_{c\alpha} \otimes r_{\alpha} \right]$$
(4)

where g denote the gravity, q the position vector, \ddot{q} its acceleration and r_{α} the contact reaction acting on the particle at the point of contact $q_{c\alpha}$. According to the additivity on internal moments in the sense of Moreau (1997), the mean stress tensor σ on the *REV* can be written as follows (5):

$$\sigma = \frac{1}{V} \sum_{p \in V} V_p \, \sigma_p \tag{5}$$

where *e* denotes the void ratio.

In (Fortin *et al.* 2003) and (Guessasma *et al.* 2006), the authors have shown the influence of dynamic effects on the mean stress tensor. Finally, the tensor σ_p is composed in three

parts: contact reaction stress, gravity stress and stress part due to the inertial forces. Accordingly, the contribution of inertial forces insures the symmetry of the stress tensor in the sense of Cauchy.

4 Modeling of fragmentation of granular material submitted to compressive stresses

The mean stress tensor presented in the previous section will be used in the modeling of fragmentation of granular material. The distribution of force chains into the granular material resulting from the compressive loading induces stress fields which are responsible of the fracture of grains. To predict the fragmentation of grain, we have considered the Mohr Theory of Failure, also known as the Coulomb-Mohr criterion or internal-friction theory (figure 3), where σ_c and σ_t are respectively the uniaxial tensile and compression strength. This theory is used in predicting the failure of brittle materials, and is applied to cases of plane stresses.

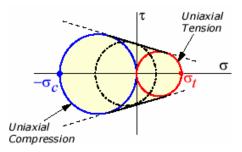


Figure.3. Coulomb-Mohr criterion

The Coulomb-Mohr criterion states that failure occurs when the two principal stresses are outside the criterion domain in the principal stress plane.

Several experimental tests using granular materials, under compressive loading, have been carried in order to understand the different fragmentation modes (figure 4a). In our case, we have considered the fragmentation mode of grains which is represented in figure 4a (Tsoungui, 1997). The corresponding numerical model is composed of 12 grains resulting from the subdivision of the initial grain.

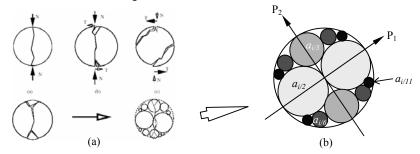


Figure.4. (a) Fragmentation modes and (b) Numerical model.

Let us consider a_i the radius of a given grain. We suppose that the Coulomb-Mohr criterion is not verified by the principal stresses into the grain for a given loading. Accordingly, the fragmentation mode of grain will be performed according to the following subdivision: the initial grain is divided in 4 gains with radius equal to $a_i/2$ and $a_i/3$, and 8 gains with radius equal to $a_i/6$ and $a_i/11$ (figure 4b).

5 Numerical simulation of oedometric test

In this part, we investigate a numerical two-dimensional model for the fragmentation of a granular material under pressure (Figure 5). The calculations are carried out with *MULTICOR* software. We consider that the behavior of granular material is perfectly rigid with density equal to 1000kg/m³ and friction coefficient about 0.2. The granular packing contains 32 grains having diameter equal to 10mm and uniaxial compression strength about 5MPa. The granular system is subjected to a pressure velocity about 0.5m/s.

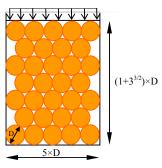


Figure.5. Oedometric test of granular packing.

The figures given below (figure 6) show the fragmentation of granular material and the corresponding forces chains distributions. The grains subjected to compressive stresses close to the uniaxial compression strength are fragmented following their principal directions. The uniaxial compression stress at the middle of the granular packing plotted with respect the time shows the evolution of stress field according the fragmentation.

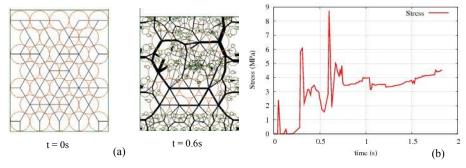


Figure.6. (a) Forces chains distributions and (b) Uniaxial compression stress.

6 Conclusion

In conclusion, we have shown that the contact force chains are crucial to the fragmentation of granular material under pressure. By considering the gravity forces after fragmentation, the rearrangement and distribution of grains seems more realistic. In addition, the overall behavior of granular material reproduces phenomena which are observed in granular media like vault effect or dilatancy.

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