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Analysis of the effect of cohesion and gravity on the bulk behaviour of powders using Distinct Element Method

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ABSTRACT

Computer simulations using Distinct Element Method have been carried out to analyse the bulk behaviour of a polydisperse assembly of glass beads. For this purpose an assembly made of 3000 spheres were generated to which the mechanical properties of glass beads were assigned.

The system was initially compressed isotropically at a strain rate of 1 s^{-1} in the absence of gravity and surface energy. Once the assembly reached a packing fraction of about 0.62, the effects of cohesion and gravity on the bulk behaviour were analysed for two different cases. In the first case only gravity was applied, whilst in the second case both gravity and surface energy were acting on the particles. The evolution of the components of the stress tensor for the case in which only gravity was applied indicated that the gravity did not appreciably affect the isotropy of the system. In contrast, the system in which surface energy was introduced became anisotropic.

The concept of unconfined yield stress of bulk cohesive powders was used to analyse the effect of surface energy and strain rate. For values of surface energy of 1.0 J/m^2 and of strain rate lower than 1 s^{-1} the unconfined yield strength did not change significantly indicating a quasi-static behaviour for the compression process. However, for values of strain rates larger than 1 s^{-1} the unconfined yield strength increased with the strain rate, following a power law trend with an index of 1.7.

1 INTRODUCTION

The processing of many particulate materials usually involves unit operations such as fluidisation, pneumatic conveying and storage in hoppers. During processing, the behaviour of powders is strongly influenced by particle properties as well as the conditions of such units. An attempt is made here to relate bulk powder behaviour under typical process conditions with single particle properties.

The flowability of powders is commonly analysed using the concept of Coulomb failure [1] as applied to the design of hoppers [2].

The influence of friction and bulk density on the quasi-static shear deformation of powders has been investigated by Thornton and co-workers [3,4]. The use of computer simulation provides access to probe the internal behaviour of particulate assemblies under mechanical loading. Therefore, the analysis of the flowability and shear behaviour of powders using computer simulation is getting increasing attention [3-5] in the recent days.

In the work reported here, computer simulations using Distinct Element Method (DEM) have been carried out to analyse the flow behaviour of powders. The analysis of the powder flowability has been carried out in terms of the unconfined yield stress.

2 SIMULATION DETAILS

An assembly of 3000 particles with properties corresponding to glass beads is considered as presented in Table 1. The particle size range is between 150 µm and 350 µm and is equally distributed in intervals of 50 µm (Table 2).

Table 1. Glass physical properties

Elastic modulus (GPa)	70
Poisson ratio	0.3
Friction coefficient	0.3
Density (kg/m^3)	2600

Table 2. Particle size distribution

Particle No.	Size (µm)
600	150
600	200
600	250
600	300
600	350

The system was formed by generating a random assembly of spheres within a cubic space and further compressing the assembly isotropically at the strain rate of 1s^{-1}. The isotropic compression was carried out in the absence of gravity and surface energy until the sample attained the packing fraction equal to 0.62. The particles deformed elastically according to the Hertz model [6] for normal contact interactions and Mindlin and Deresiewicz [7] and Thornton and Randall [8] for tangential contact interactions. When surface energy was assigned to the particles in contact the models of Johnson *et al.* [6] and Savkoor and Briggs [10] were used to determine the normal and tangential contact force respectively.

During compression the variation of the stress tensor (stress ratio) were obtained to analyse the stress transmission characteristics within the system [3]. The components of the stress tensor are defined as

$$\sigma_{ij} = \frac{2}{V}\sum_{1}^{N} RNn_i n_j + \frac{2}{V}\sum_{1}^{N} RTn_i t_j \qquad (1)$$

where Rn_i is the *i* component of the radius vector from the centre of the particle to the contact and Nn_i, Tt_j are the *i* and *j* components of the normal and tangential contact forces and *N* the number of interparticle contacts. The stress ratio, σ_R, is defined as:

$$\sigma_R = \frac{\sigma_{ii} - \sigma_{jj}}{\sigma_0} \qquad (2)$$

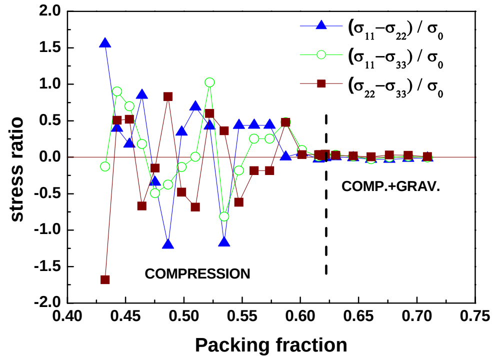
3 RESULTS

3.1 Effect of gravity and surface energy on the stress ratio

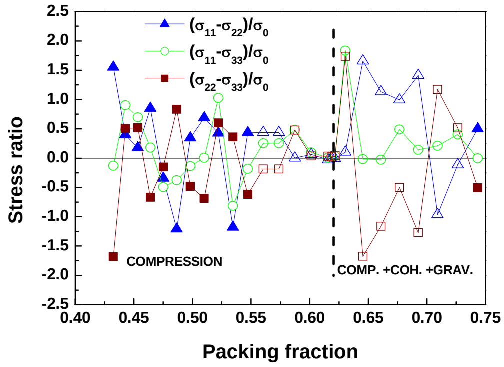
The effect of gravity and surface energy has been analysed by introducing these effects once the assembly reached the packing fraction equal to 0.62. Two different cases have been considered. In the first case only gravity was introduced. In the second case gravity and surface energy were assigned to the particles simultaneously.

The evolution of stress ratios with packing fraction is presented in Fig. 1a-b. The stress ratios show a high anisotropy for assemblies with packing fraction less than 0.60. However, for larger values of packing fraction the system becomes isotropic, suggesting an un-bias in he force network acting within the assembly.

Fig. 1a clearly indicates that the introduction of gravity does not affect the isotropy of the system appreciably. In contrast, the introduction of surface energy at the value of 1.0 J/m^2 produces oscillations in the stress ratios indicating that the isotropy of the system have been broken.



a)



b)

Figure 1: Evolution of the stress tensor with packing fraction in the presence of: a) only gravity and b) gravity and surface energy (1.0 J/m^2) were introduced.

The pull-off force, F_{OFF} or force required to break an adhesive contact between two particles of radii, R_1 and R_2, is given by

$$F_{OFF} = 3\pi\gamma R \qquad (3)$$

where $R^{-1} = (R_1^{-1}+R_2^{-1})$ is the reduced radius of two particles in contact and γ is the surface energy. When surface energy is introduced at the value of 1.0 J/m^2 the pull-off force has the value of 1.6 mN for the largest particles which is significantly larger than the particle weight (about 4.6 μN). Therefore, a larger influence of the interparticle interaction could be expected as confirmed by the results plotted in Figs. 1a-b.

3.2 Effect of surface energy on the flowability of powders

The flow properties of particles are usually measured by using direct or indirect shear testers [12]. In the study carried out here, as performed in the industry, the flowability of powders is analysed by measuring the unconfined yield stress by performing an uniaxial compression test [12] (Fig. 2). This test is performed in a similar way to the experimental one. Once the sample has been formed and consolidated (for two different values of surface energy) an infinitely rigid platen is introduced as the bottom boundary of the assembly as shown in Fig. 2. An elastic platen (steel) was positioned near the top of the sample and later moved downwards with a specific strain rate.

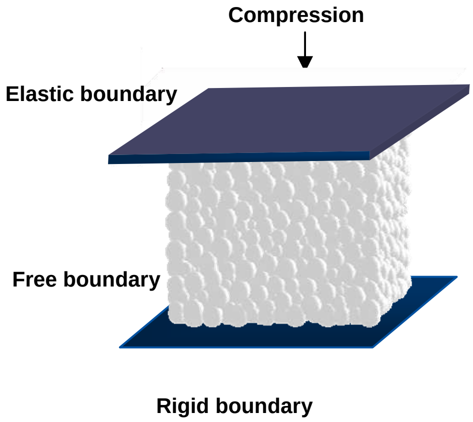


Figure 2: Schematic diagram of the test for measuring the unconfined yield stress.

The number of interparticle contacts as well as the force acting on the top platen was monitored during the compression. The sample was considered to have failed when a sharp peak in the platen force accompanied by a significant drop in the number of contacts was observed.

Figure 3 shows in log-log scale the unconfined yield stress (UYS) as a function of the strain rate for the cases of particles with surface energy 0.1 J/m^2 and 1.0 J/m^2. The UYS does not depend on strain rate for values of strain rate lower than 2s^{-1} for the system with 0.1J/m^2 and lower than 6 s^{-1} for the case of system with surface energy 1.0 J/m^2. It is noticed that an increase of one order of magnitude in the surface energy produces an increase of one order of magnitude in the UYS for the quasi-static regime. This indicates a decrease in the flowability of powders when the surface energy increases.

For large values of strain rate a power law relationship between UYS and strain rate, γ, is observed. The power law index is equal to 1.7.

A power index of less than two suggests that the pressure originated in the system is not exclusively due to a kinetic contribution as observed in the case of rapid granular flows but due to the influence of the interparticle friction. This behaviour is typical of systems with large values of packing fraction and corresponds to an intermediate regime between quasi-static and rapid granular flow as suggested by Tardos *et al.* [13].

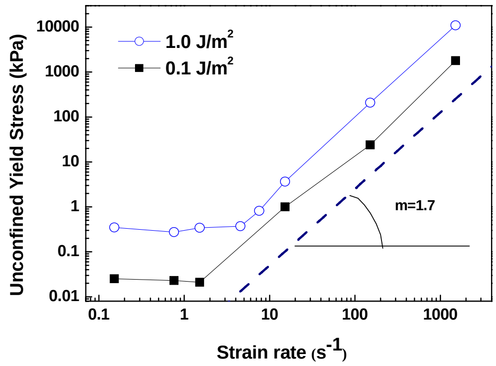


Figure 3: Unconfined yield stress as a function of the strain rate for two different values of the surface energy of the particles.

In the simulations reported here the particles are only allowed to deform elastically and neither plastic deformation nor particle breakage or air effects have been considered in our simulations. This imposes a limit on the significance of the data at very high strain rates.

4 CONCLUSIONS

The effect of isotropic and unconfined compression on the behaviour of a bulk of cohesive particles has been investigated by using Distinct Element Method.

When the system was subjected to an isotropic compression and for low values of packing fraction, the stress ratios showed a high anisotropy of the contact forces. In contrast, when the packing fraction increased, the system became isotropic. Once the assembly of particles reached a high value of packing fraction (0.62) the influence of gravity and surface energy on the contact forces was analysed. The introduction of gravity in the system did not appreciably change the variation in stress ratios. However, oscillations of the stress ratios indicating an anisotropic force propagation were observed when surface energy was introduced in the system.

The analysis of the flowability of the powders was carried out by quantifying the unconfined yield stress. An increase of one order of magnitude in surface energy produced an increase of one order of magnitude in the unconfined yield stress.

Furthermore, the limit between quasi-static and non-quasi-static regime extended for larger values of strain rate in the case of particles having larger surface energy (1.0 J/m^2). These results highlighted the importance of the interparticle interaction on the bulk behaviour of cohesive powders.

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