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Crack nucleation and propagation in rounded cohesive granular media

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Abstract. This work investigates the influence of cohesion on aspects of fracture mode and propagation in 2D rounded cohesive granular packing. Simulations are undertaken using the molecular dynamics method involving simple contact laws with adhesion. The numerical “Brazilian” test with samples of 8000 circular particles suggests that the formation of crystallized agglomerates within mono-disperse samples depends on the value of the cohesive energy between particles. The agglomerate size is increased when the surface energy increases. In the testing phase and for high values of surface energy, the fissures appear at the agglomerate interfaces in the center of sample and propagate toward the periphery in parallel to the compressive direction.

Keywords: Granular material, adhesion, molecular dynamics, crack, agglomerate

1. Introduction

Granular materials may be considered as an assembly of particles of differing size, the macroscopic behavior of which is governed by interactions between particles. In civil engineering work, natural or reshaped soil can intervene in the construction of foundations, dams or underground structures, Granular substances are used in the fabrication of concrete and also occur in fragmentation processes. In the agro-product, pharmaceutical and chemical industry, many products are constituted from grains or powders. The prediction of the stability of structures in geo-materials, and the collapse, transportation and stocking of granular materials are problems involving the mechanic behavior of granular materials. The macroscopic and microscopic properties of granular media are complex. Many experimental and numerical studies on the mechanical behavior of granular packing have been undertaken over the last twenty years, with the aim of predicting the macroscopic behavior of granular media and investigating the grain scale or the contact scale. These studies indicate that if the whole medium is dense, it is then very strongly structured. This conclusion was first made from the contact force network analysis of inhomogeneous nature [7], and secondly from the study of the contact directions which characterize the nonisotropy of the contact network [2,3,5]. However, these investigations concern only the non-cohesive granular media.

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The aim of this work is to quantify, by numerical simulation, the influence of cohesion on the aspect of fracture and the crack propagation of the systems by progressively increasing the surface energy (adhesion) between particles, starting with a non-cohesive medium. In this paper, we first present a simple model of adhesion between two circular particles. After a short description of the numerical sample and of the boundary conditions, we present our main results regarding the agglomerate size, the average coordination number and the contact directions in the equilibrium state and the crack propagation in the testing phase as a function of surface energy between contacts.

2. Adhesion in molecular dynamics simulations

The simulations were carried out on 2D numerical samples using the Molecular Dynamics (MD) method based on the predictor-corrector scheme with Gear's set of corrector coefficient for the integration of Newton's equation of motion [1]. In molecular dynamics or most popular discrete element simulation methods, the particles are handled as rigid bodies. In our numerical algorithm, we introduced a model of adhesion between two particles in contact characterized by the relative displacement of the particles centers from the "just at contact" position (an overlap δ) and a contact surface $2a$; (Fig. 1). To a first order approximation in δ/r , the radius of the contact zone is given by $a = \sqrt{r\delta}$.

In our work, we consider firstly the normal effect of adhesion on contact. The adhesion is introduced as a contact resistance to a separation effort. With an idea similar to the adhesion model on solid surface of JKR [4], we established an interaction model between two particles in which the contact force is the sum of a repulsive force proportional to an overlap δ , and an attractive force proportional to a contact surface $2a$. In the retained model and in a quasi-static approximation, the repulsive force depends on a contact stiffness k , given by $k\delta$, and the attraction force on an adhesive energy γ , given by $\gamma\sqrt{r\delta}$. The dynamic effects are taken into account by viscous damping term $\alpha\dot{\delta}$, where α represents the normal damping coefficient and $\dot{\delta}$ the relative velocity. So the expression for normal force of contact F_n is a function of δ given by [6,8]

$$F_n = k\delta + \alpha\dot{\delta} - \gamma\sqrt{r\delta}. \quad (1)$$

With regard to the tangent force, we choose a Coulomb's type friction law but with a modification to account for the fact that the contact can support tensile force (Fig. 2). Since the integration of movement

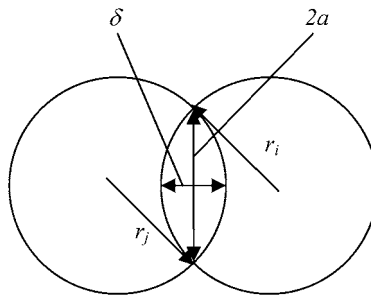


Fig. 1. Geometry of the contact between two disks.

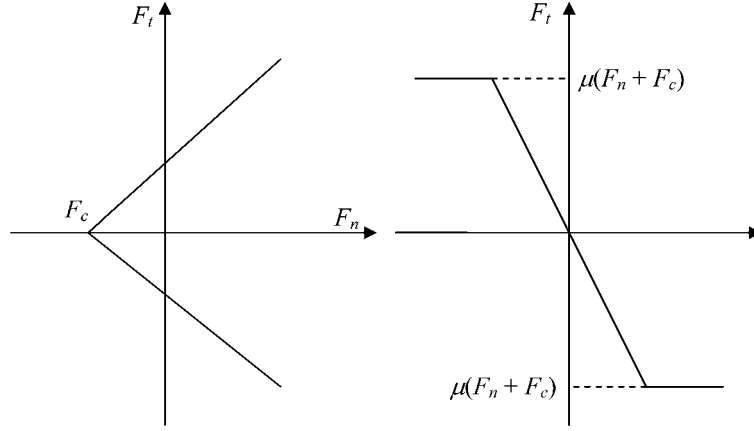


Fig. 2. Regularized Coulomb's law of friction with adhesion.

equations requires a regular friction force, we implemented the regularized Coulomb's law with adhesion given by this expression [6,8]

$$F_t = \min\{|\gamma_s v_s|, F_c\} \cdot \text{sign}(v_s), \quad (2)$$

where γ_s represent the tangential viscosity and v_s relative sliding velocity. Note that in the present model, the overlap is permitted. This overlap can be interpreted in term of the interaction zone or of the particle deformation. A force law with adhesion in a broad sense involves a pair of adjacent particles that resist not only normal separation, but also relative sliding and rolling. When these conditions are fulfilled, the interparticle contact is "cemented", i.e. the relative degree of freedom of particles in contact is frozen within the range of supportable forces and moments. However, we will not consider here the rolling friction and stiffness so that contiguous particles may freely roll on one another with no bending moment acting between them.

3. Numerical samples

Numerical 2D samples are considered, composed of 8000 circular particles. Two granular systems were simulated. One consists of disperse particles with the radius of 3 mm (mono-disperse system) and in the other system the particle radii are uniformly distributed between 2 and 4 mm (poly-disperse systems). For preparing a well compacted circular sample, we utilized a simple technique in which the particles are distributed randomly in a triangular network without contact in a circular box. The radius of the circular box is then reduced until the available space is fully occupied, and the system is under compression in all directions. Gravitational effects are neglected. When the particles fill the space and these are then rearranged until a static equilibrium is reached. The adhesion between the rounded box and the particles is zero. The surface energy γ is prescribed at contact level for each simulation. The stiffness and the coefficient of damping are the same for all particle-particle and particle-box contacts. The next step involves the release of the sample by slowly increasing the rounded box radius to allow the system to relax to a static equilibrium again. The final state of this preparation step is used as the initial equilibrium state for the analysis and for the Brazilian test. This test is often used to determine the resistance to tensile force of materials which do not support tensile loads well, such as concrete. The

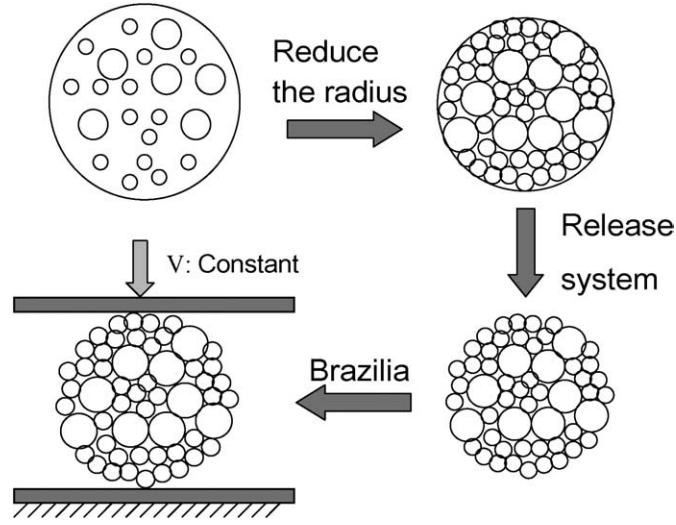


Fig. 3. Sample preparation under stress by reduction of the rounded box radius and the Brazilian test scheme.

Brazilian test is realized by placing the sample between two flat plates (Fig. 3). In the simulation, there is no adhesion between the particles and the flat plates but all other parameters of particle-flat plate contact are the same values for particle-particle contact. The lower flat plate is fixed while the upper plate is pushed down (direction $-y$) with a constant velocity of displacement. The numerical simulations are stopped when the macroscopic strain in the y direction reaches approximately 10%.

4. Numerical results

4.1. Initial equilibrium state

A significant feature of our simulation results is the formation of agglomerate regions in the sample. For the mono-disperse system, we observe that the structure forms crystallized zones and agglomerates, the sizes of which increase with the adhesion γ . The formation of agglomerates is clearest from the images showing local coordination number (Fig. 4 upper). The structure is also clarified in the image that reflects interaction forces and we can see the low stress joins (white colour) which form the interfaces of the agglomerates (Fig. 4 lower). In contrast for the poly-disperse system, the formation is not clear for all values of adhesion γ (Fig. 5). Moreover, for two granular systems, we found that the coordinate number or the average number of contacts per particle is lower than 4 for low values of adhesion ($\gamma < k/50$), similar to non-cohesive granular media, but exceeds 4 for high values of adhesion.

In the mono-disperse systems which are composed of some agglomerates, the structure arranges the contacts in 3 principle directions as we can see from the histogram of the contact direction (Fig. 6a). Contrary to the poly-disperse sample, we observe that the contacts are distributed in a quasi-isotropic way for all adhesion values, without any dominant directions (Fig. 6b).

4.2. Crack mode and propagation

The investigation of crack mode and propagation is carried out by the Brazilian test, starting from samples in the initial equilibrium state. Of course, the ultimate failure load of the system increases when

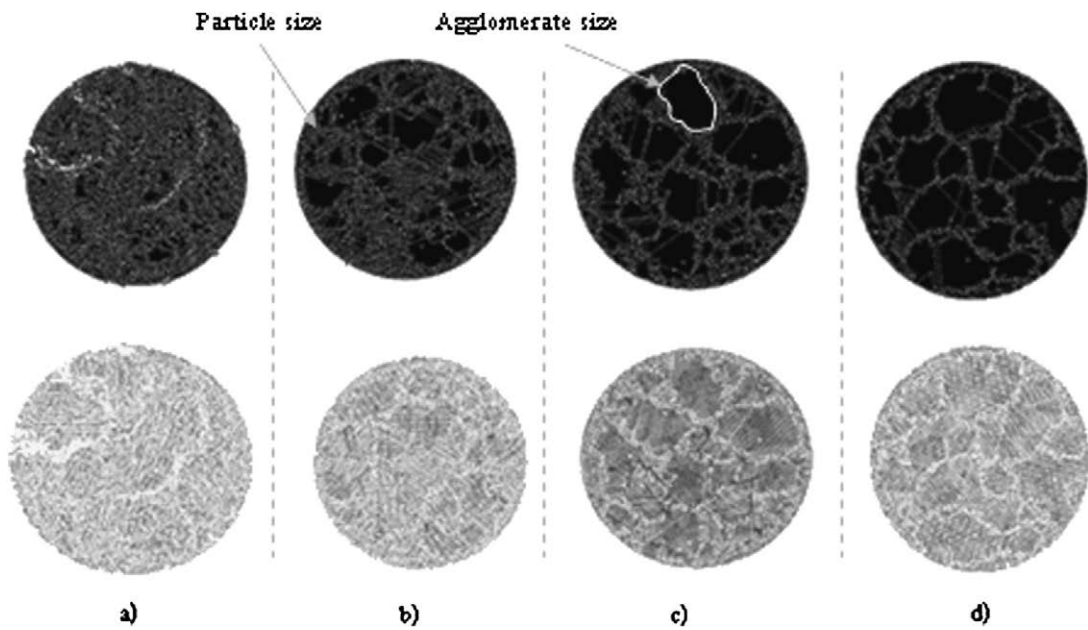


Fig. 4. In mono-disperse systems (upper) local coordination number coded in greyscale (6 contacts in black, 5 in dark grey, 4 in bright grey and white for less than 4); (lower) normal contact force network of initial equilibrium state of sample with $\mu = 0.5$ for four different values of adhesion: $\gamma = k/150$ (a), $\gamma = k/50$ (b), $\gamma = k/20$ (c) and $\gamma = k/7$ (d). The compressive forces in contact are traced in black and the tensile forces in grey.

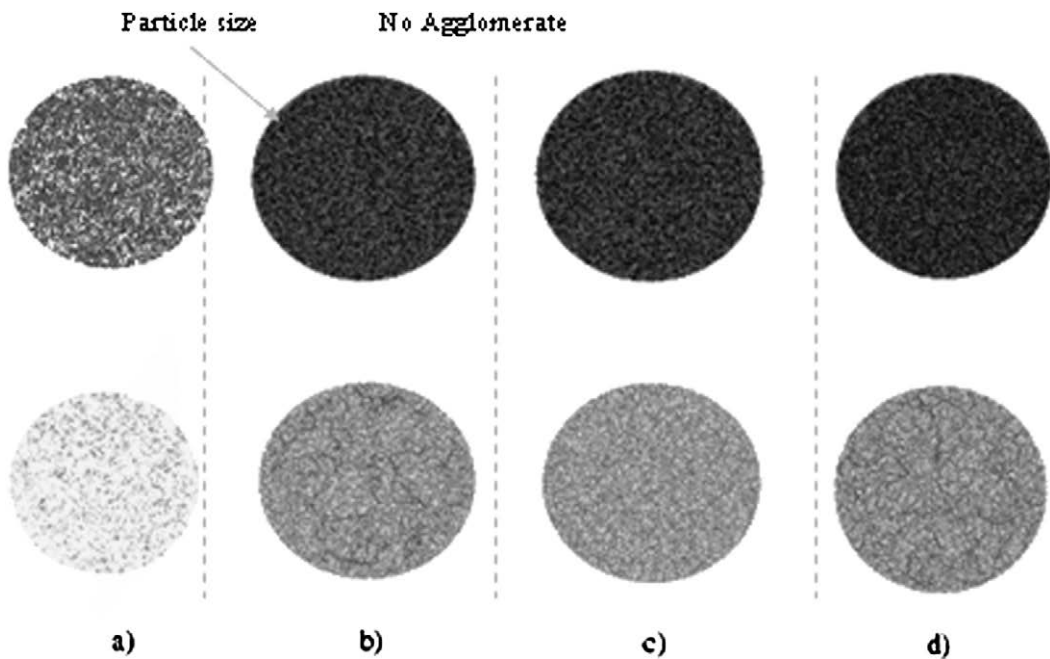


Fig. 5. In poly-disperse systems (upper) local coordination number coded in greyscale (6 contacts in black, 5 in dark grey, 4 in bright grey and white for less than 4); (lower) normal contact force network of initial equilibrium state of sample with $\mu = 0.5$ for four different values of adhesion: $\gamma = k/150$ (a), $\gamma = k/50$ (b), $\gamma = k/20$ (c) and $\gamma = k/7$ (d). The compressive forces in contact are traced in black and the tensile forces in grey.

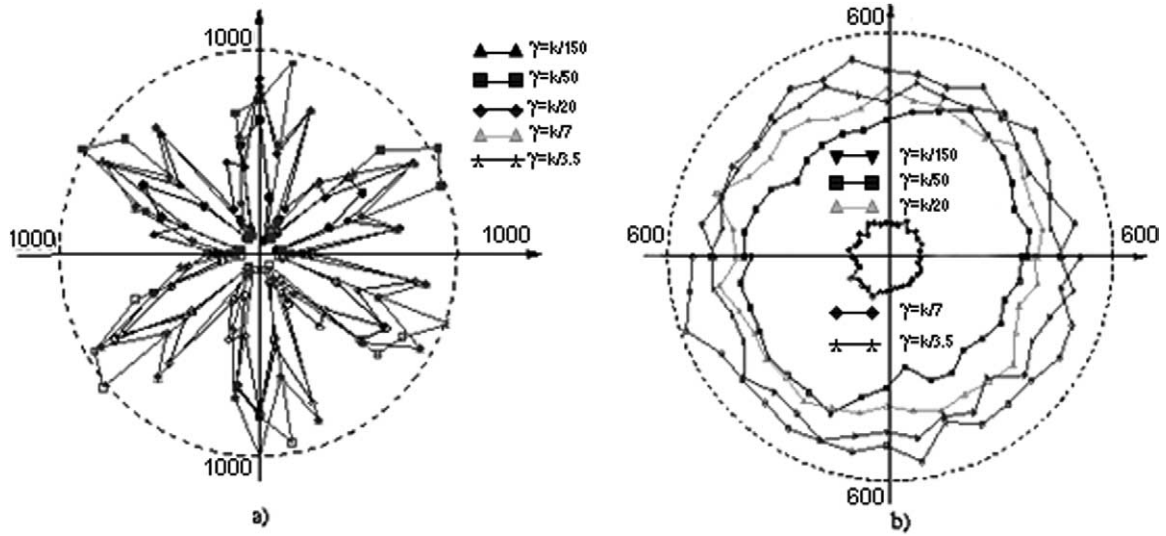


Fig. 6. Polar diagram of the distribution of the number of contacts for repulsive (upper) and tensile (lower) contacts for (a) mono-disperse systems and (b) poly-disperse systems.

the local surface energy between particles increases. We observe that faults appear and are manifested near the circumference for low values of adhesion for both systems. In contrast, for high values of adhesion of both granular samples, the first fissure occurs at the centre of the sample and propagates throughout the periphery (Fig. 7). This high cohesive behaviour reconciles the results of elasticity theory in which the tensile stress is maximum at the centre of the sample [9]. Otherwise, the fissure is oriented in a vertical direction, corresponding to the maximum stress direction in compression. These figures show also that the medium tend to form a lump structure for high cohesive systems. In the less cohesive cases the medium was found to break into a crumble-like structure.

A particular aspect of the fissures, in the mono-disperse systems, is their initiation and propagation in the agglomerate joints where the structure is less compact. It is also seen that the initial agglomerate remains intact. This result is confirmed by the evolution of contact directions (Fig. 8). The compression contacts are oriented and increased in the applied stress direction, whilst the traction contacts are rearranged in the orthogonal direction. Nevertheless, this evolution doesn't damage the favored orientation which is dominated by the structures connecting the triangular network inside the agglomerates.

5. Conclusion

The result of the numerical investigations described demonstrates the feasibility of the indirect tensile test as a simulation tool. We can obtain the auto-equilibrium geometry of enough regular form. The choice of a homogeneous system allows samples to be generated that present a disorderly type "joints of agglomerate" and to observe that the weak effort or contact zones which guide the fissure and fracture of the medium. A uniform distribution particle radii help to create a quasi-isotropy material. The values of adhesive energy between particles change the macroscopic behaviour, in particular the crack mode and propagation. The investigation presented here could be extended for characterizing an evolution of stress in the ruin phase of a structure.

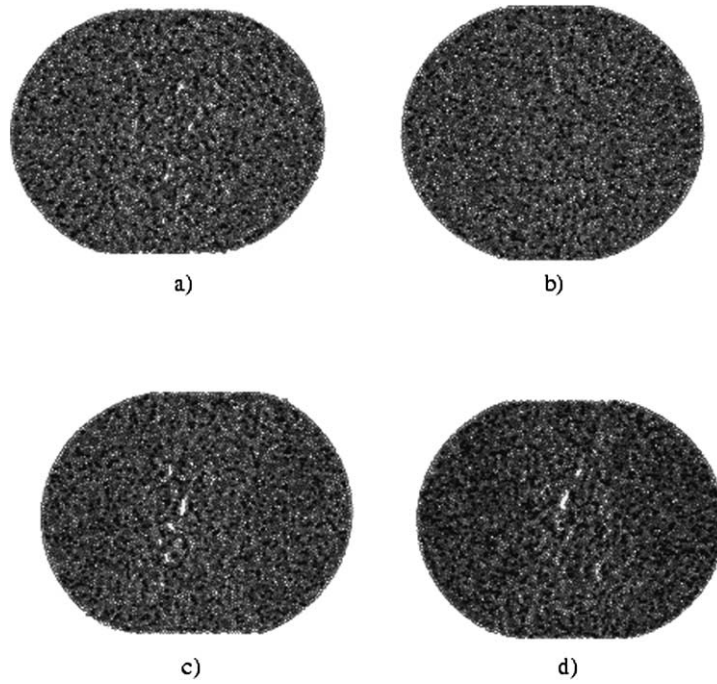


Fig. 7. Configuration of the sample for poly-disperse systems at 10% of macroscopic strain for four values of adhesive energy: (a) $\gamma = k/20$, (b) $\gamma = k/10$, (c) $\gamma = k/7$ and (d) $\gamma = k/3.5$. The greyscale represents the coordination number: black for 6, dark grey for 5, bright grey for 4 and white for less than 4.

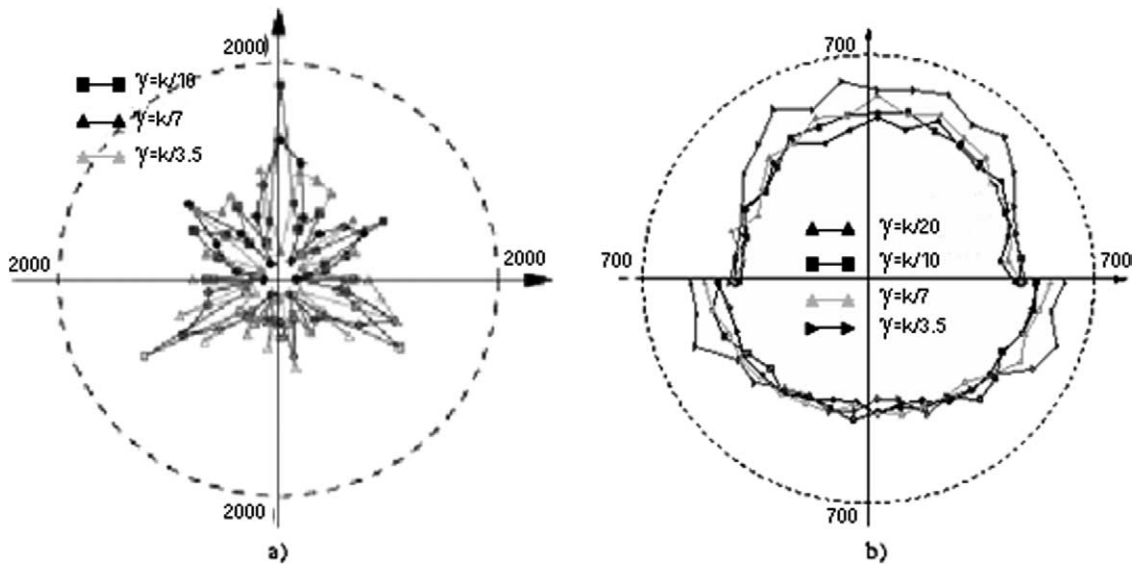


Fig. 8. Polar diagram of the distribution of the number of contacts at 10% of macroscopic strain for repulsive (upper) and tensile (lower) contacts for (a) mono-disperse systems and (b) poly-disperse systems.

Acknowledgements

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