Influence of the grains shape on the mechanical behavior of granular materials

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Abstract. Discrete Element Method is a numerical method suitable for modeling geotechnical problems concerning granular media. In most cases simple forms of grains, like discs or spheres, are used. But these shapes are capable of soil behavior modeling up to a certain point only, they cannot reflect all of the features of the medium (large shear resistance and large volumetric change). In order to reflect the complex behavior of the real soil either other grain forms or numerical parameters have to be used. The question of shape influence has not been fully understood yet. The aim of the present paper is to study the influence of the grains shape on the mechanical behavior of granular assemblies, grains convexity in particular. Two groups of grains are compared: convex irregular polygons, and non-convex clumps of three overlapping disks. These shapes are chosen because of the similarity of global shape. A large number of shape variants was used in both groups and a shape parameter α is introduced. The samples were loaded in a vertical compression test simulated with a 2D DEM code. The results are investigated on both macro- and microscopic levels. Evident differences in the behavior of two particle groups are studied and discussed: convexity influence on macroscopic friction angles values, different mechanisms of shear localization. It appears that assemblies of clumps lead to shear band forming while assemblies of polygons lead to diffused rupture mechanism.
This work was done as a part of CEGEO research project[1].

Keywords: DEM, grain shape, clump of discs, polygon, 2D vertical compression, shear strain localization
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INTRODUCTION

Using a Discrete Element code, series of numerical simulations have been performed on 2D granular material composed of clumps made of three overlapping discs and polygonal particles of six edges. Performing vertical compressions the influence of grain shapes is studied. In this paper we shortly describe the numerical procedures of the test. Then, we present some observations of dense and loose granular assemblies under an isotropic loading. The mechanical responses of vertical compression tests are compared for various grain shapes. Finally, we discuss the kinematics of the deformed granular assemblies.

TABLE 1. α values for polygons and clumps

Polygons	-	-	0.13	0.18	0.20	0.21
α	0.24	0.26	0.28	0.30	0.40	0.50
Clumps	0.00	0.10	-	-	0.20	-
α	-	-	-	0.30	0.40	0.50

[1] www.granulo-science.org/CEGEO

GRANULAR MODEL

The considered granular model is a 2D assembly of 5000 polydisperse frictional particles, whose surface areas are uniformly distributed and whose radii respect a relation $R_{max} = 3R_{min}$.

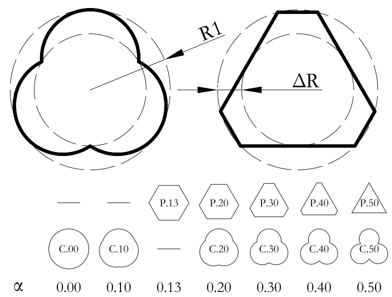

FIGURE 1. Particle shapes used and sample names

A shape-defining parameter $\alpha = \frac{\Delta R}{R_1}$ was introduced, where R_1 denotes the grain excircle radius and ΔR is the difference between the ex- and the incircle (Fig.1). For convex polygonal grains α range is from 0.13 ($\simeq 1 - \frac{\sqrt{3}}{2}$; regular hexagons) to 0.5 (equilateral triangles). For non-convex clumps α ranges from 0 (circle) to 0.5. All the samples used were presented in Tab.1. Four different samples of each α value was used.

DISCRETE ELEMENT METHOD

The study was done using Discrete Element Method in the framework of Molecular Dynamics principles. Normal contact forces were computed using a linear elastic law $f_n = k_n \cdot h$. Tangential forces were computed using Coulomb friction law: $f_t = \pm\mu \cdot f_n$. Motion laws used were drawn from Newton's equations and integrated with a third orded predictor-corrector scheme [1]. Contact detection for clumps was solved as for disks: a contact occurs in a point, the normal force value f_n is computed basing on the overlap distance h and its direction connects the centres of disks in contact (Fig.2). For polygons *Shadow Overlap* technique developed by J.-J. Moreau was used [2]. The main difference between it and the classical approach is that here we introduce two contact points at every edge-to-edge contact instead of one and the force value is computed proportionally to the overlap distance h. Polygonal particles can engage in two types of contacts: corner-to-edge and edge-to-edge. By analogy with these two types, four possible contact types for clumps were divided into two groups (Fig.2). This has an influence on coordination number values, discussed later.

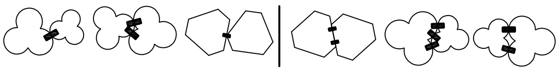

FIGURE 2. Contact types for clumps and polygons: *corner-to-edge* (left) and *edge-to-edge* (right)

The normal stiffness of contact was computed according to the dimensionless 2D *stiffness parameter* $\kappa = k_n/\sigma_3$ [3]. Its value was arbitrary set to 1000. Mean overlap of particles is proportional to the relation $1/\kappa$. Values of normal and tangential contact stiffnesses were assumed to be equal, $k_n = k_t$.

OBSERVATIONS IN STATIC LOADING

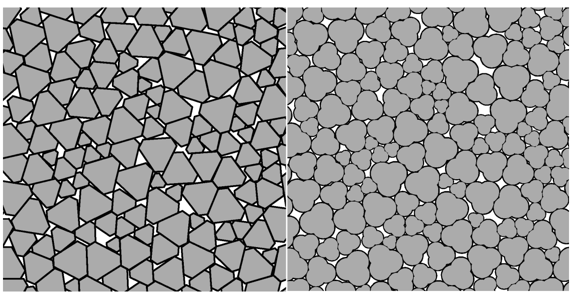

FIGURE 3. Samples fragments with $\alpha = 0.3$ in the isotropic state.

Behavior of the granular assembly is mainly driven by the initial configuration of the particles, as observed already by [4]. To ensure the homogeneity of contact network and void spatial distribution, the samples were prepared in steps: first the grains were randomly distributed inside a square made of four rigid walls, next grain growing phase started and finally the samples were isotropically loaded up to $\sigma_3 = 10kPa$, which took around 50000 timesteps. During these preparations, in order to obtain dense samples, intergranular friction coefficient μ was equal 0, while $\mu = 0.5$ was used to create loose ones. To investigate the initial state of the samples in the isotropic state we studied *coordination number* z^*, which corresponds to the mean contact number per grain in the sample (only grains that support at least two compression forces are considered). The values of z^* are very similar for clump and polygon samples (Fig.4). In every figure clump samples are marked with circles and polygon ones with polygons. Dense samples are signified by black symbols, loose ones by white.

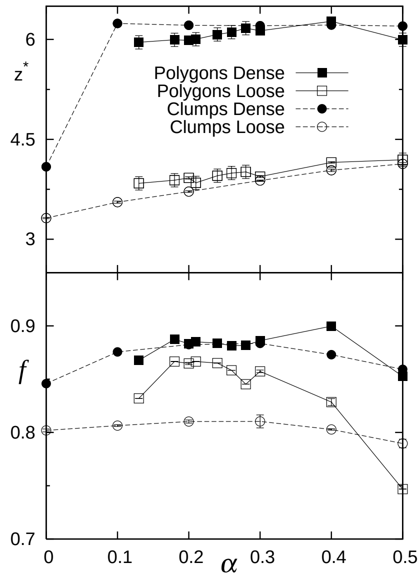

FIGURE 4. Coordination number z^* and compacity f values vs. α under an isotropic loading. Errors bars correspond to standard deviation computed over a population of four samples. round symbols: clumps; blacks symbols: dense samples

Dense samples show constant values of z^* for all the shapes, while in loose samples z^* values are increasing along with α. Compacity evolution clearly show that within the chosen method of preparation polygons tend to create denser assemblies than clumps.

MECHANICAL BEHAVIOR UNDER VERTICAL COMPRESSION

The samples were tested in a 2D strain controlled vertical compression test. In order to assure the similitude of the tests, loading velocities were chosen according to the *inertial number* $I = \dot{\varepsilon}_1\sqrt{\frac{\langle m\rangle}{\sigma_3}}$ [5], which value was set to

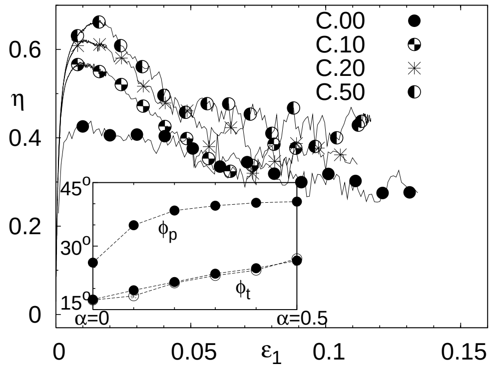

FIGURE 5. $\eta - \varepsilon_1$ curves for some dense clump samples; Subfigure: friction angles evolution for all clump samples

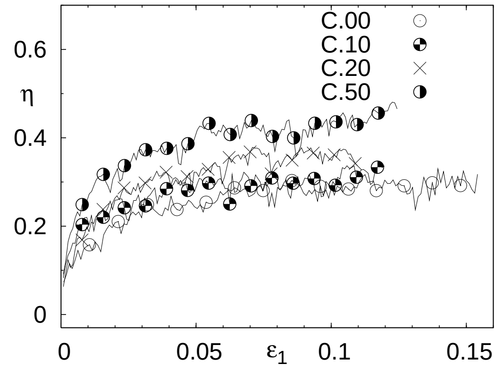

FIGURE 7. $\eta - \varepsilon_1$ curves for some loose clump samples

$5 \cdot 10^{-5}$ and where $\dot{\varepsilon}_1$ denotes the strain rate and $\langle m \rangle$ is the mean mass. The macroscopic results of tests are plotted on η vs. ε_1 charts, where $\eta = \frac{t}{s}$, $t = \frac{\sigma_1 - \sigma_3}{2}$ and $s = \frac{\sigma_1 + \sigma_3}{2}$. When comparing stress-strain curves (Fig.5-8) it is clear that for clump samples both peak ϕ_p and threshold ϕ_t friction angle values increase along with α (Fig.5). On the other hand, in polygon samples ϕ_p values decrease with α, while ϕ_t values increase (Fig.6). For samples made of equilateral triangles ($\alpha = 0.5$) the two values are almost equal. For loose samples there is no peak value of the friction angle. We observe a peak in some of the loose polygon samples.

There is no particular influence of particle convexity on average dilatancy angle ψ values ($\sin\psi = \frac{d\varepsilon_1 + d\varepsilon_3}{d\varepsilon_1 - d\varepsilon_3}$) of clump samples, both dense and loose (Fig.8). On the other hand, ψ is lower for polygons with higher values of α than for the ones more similar to hexagons. Moreover, polygon samples show bigger overal dilatancy than samples made of clumps. Values of dilatancy angles for dense samples were computed at the peak, between [1,5 - 2,5%]ε_1; For loose ones the range was [6 - 7%]ε_1.

MICROMECHANICAL ANALYSIS

At the end of the tests ($\varepsilon = 12\%$) intergranular contact proportions are investigated. The percentage of corner-to-edge contacts is much higher than edge-to-edge ones (Fig.9) and does not depend on the initial sample compacity (Fig.4). On the other hand, the proportions of contacts are correlated with the shape of grains, as for higher values of α the percentage decrease in clump samples. Similar trend was observed with the macroscopic friction angle values and discussed in previous section. The tendency is not clear in polygon samples.

In order to study the kinematic origins of macroscopic rupture, we choose to focus on the strain localization in the samples. Two approaches are used for that: *local strain maps* and *Shear localization Indicator* S_2 [6]. Using particle kinematics from the isotropic state to a

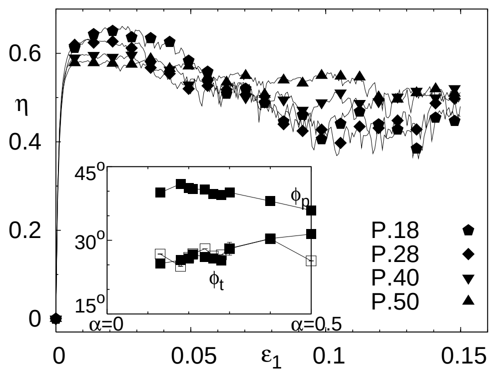

FIGURE 6. $\eta - \varepsilon_1$ curves for some dense polygon samples; Subfigure: friction angles evolution for all polygon samples

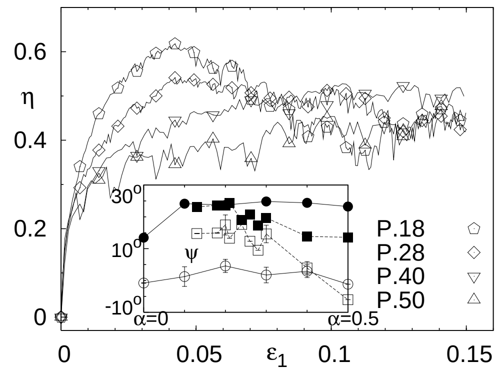

FIGURE 8. $\eta - \varepsilon_1$ curves for some loose polygon samples; Subfigure: dilatation angles evolution for all the samples

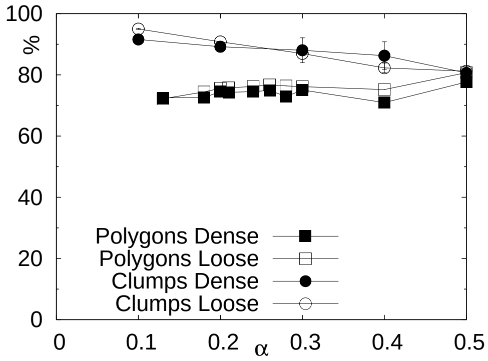

FIGURE 9. Corner-to-edge contacts percentage at the end of the vertical compressions.

deformed stage, local strains are computed like [7] over Delauney triangulation. Figure 10 use the second invariant of the strain tensor to illustrate the shear localization.

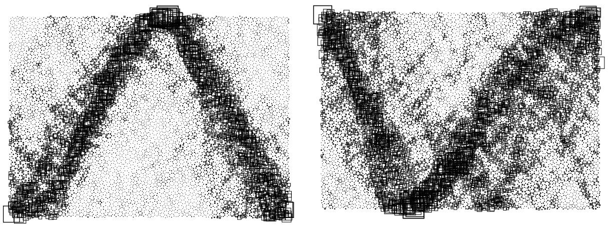

FIGURE 10. Shearmaps: dense clump (left) and polygon (right) samples with $\alpha = 0.3$. $\varepsilon_1 = 0 - 13.5\%$

These shear maps shows that polygon samples create wide shearbands that develop slowly during the test, contrary to clumps, where localization zones are narrower and appear rapidly, probably due to the grain imbrications. This complies with the previous remarks about the overall dilatancy of the samples.

The definition of shear localization indicator is $S_2 = \frac{1}{N_t}\left(\sum_{i=1}^{N_t} I_{2\varepsilon}\right)^2 / \left(\sum_{i=1}^{N_t} I_{2\varepsilon}^2\right)$ where $I_{2\varepsilon}$ is the second invariant of the strain tensor and N_t is the total numbers of triangles. Value of S_2 can be regarded as a percentage of a sample surface that has been distorted. Figure 11 give the evolution of S_2 for several samples made of clumps and polygons: close to the isotropic state both groups behave similarly and the maximum value of S_2 is reached at about 2% of ε_1. At this stage at least 50% is deformed. After, S_2 decreases, which indicates that $I_{2\varepsilon}$ localise in a focused zone. For dense samples this zone is smaller for clumps than for polygons and appears for lower ε_1. What is more, the shape of S_2 curves is closely correlated with the shape of stress-strain curves. The peak positions and its widths overlap precisely. The threshold values of S_2 are $10 - 20\%$ higher for polygon samples than for clumps of the same α. Apart from the two localization mechanisms described above, loose clump samples and the loose ones made of polygons with $\alpha = 0.4$ and 0.5 do not localise strains at all (S_2 value increases up to 60% during the tests). Submitted to biaxial tests, polygon samples slowly create wide shearbands and thus resemble soil behavior. Clumps behave more like a brittle material, shear bands are thin are their expansion is quick. These kinematic differences comes essentially from geometrical imbrications of clumps where concavity is involved.

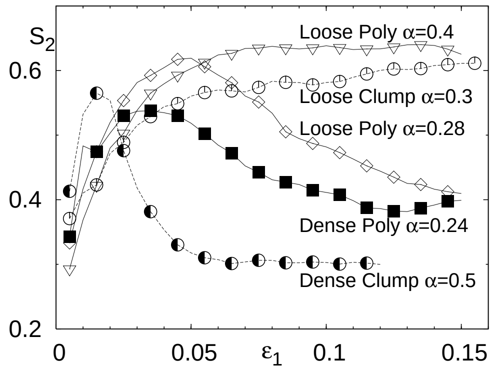

FIGURE 11. Shear indicator evolution during a vertical compression

CONCLUSIONS

Studying the mechanical response of granular samples submitted to vertical compression, samples made of clumps (non-convex grains) or made of polygons show different behavior. Whereas clump concavity increase shear resistance, the effect of changing polygons shapes via α is less spectacular. Focusing on the kinematics involved in shear localisation, dense samples made of polygons show realistic features of cohesionless granular soils. The authors tend to connect these facts with the influence of intergranular contact types and grains imbrications, but the theory needs more investigation still.

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