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Systematic description of the effect of particle shape on the strength properties of granular media

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Abstract. In this paper, we explore numerically the effect of particle shape on the mechanical behavior of sheared granular packings. In the framework of the Contact Dynamic (CD) Method, we model angular shape as irregular polyhedral particles, non-convex shape as regular aggregates of four overlapping spheres, elongated shape as rounded cap rectangles and platy shape as square-plates. Binary granular mixture consisting of disks and elongated particles are also considered. For each above situations, the number of face of polyhedral particles, the overlap of spheres, the aspect ratio of elongated and platy particles, are systematically varied from spheres to very angular, non-convex, elongated and platy shapes. The level of homogeneity of binary mixture varies from homogenous packing to fully segregated packings. Our numerical results suggest that the effects of shape parameters are nonlinear and counterintuitive. We show that the shear strength increases as shape deviate from spherical shape. But, for angular shapes it first increases up to a maximum value and then saturates to a constant value as the particles become more angular. For mixture of two shapes, the strength increases with respect of the increase of the proportion of elongated particles, but surprisingly it is independent with the level of homogeneity of the mixture. A detailed analysis of the contact network topology, evidence that various contact types contribute differently to stress transmission at the micro-scale.

1 Introduction

In many particulate materials found in nature and industry, scientists and engineers need to quantify the effect of complex particle shapes. This is of major importance in the context of civil engineering and powder technology, where most processes need to be optimized or revised following the dramatic degradation of natural resources. Non-convex particles can be found in metallurgical and sintered powders, angular shaped particles are common in rocks and soils, whereas elongated and platy particles may occur in pharmaceutical and food products. Mixture of shapes is also used in order to reinforce soils or in civil engineering structures.

The first works dealing with particles shape parameters are not new. Indeed authors such Wadell in 1932 [1] or Krumbein Pettijohn 1938 [2] are the first to have developed methods for characterizing the shape of the particles.

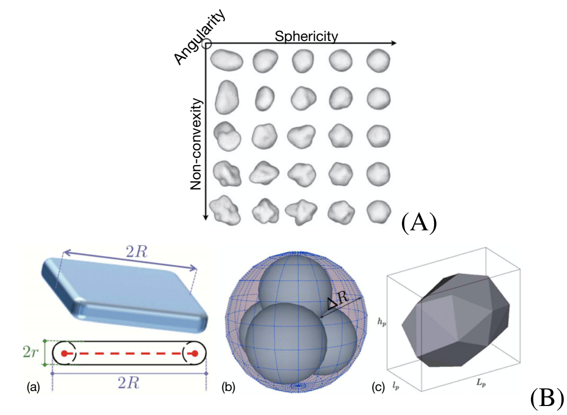

Figure 1. (A) 3D-diagram of particles shapes following Santamarina [3]. (B-a) Platy (elongated in 2D), (B-b) Non-convex and (B-c) Angular shapes .

These methods were primarily dedicated to the characterization of particles in the field of Sedimentology. Without going into details of the classification techniques, the particles can be grouped into three categories according to their angular, non-convex or elongation/platyness (also called sphericity) nature; see Figure 1(A).

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Nevertheless, even if an increasing number of experimental and numerical studies have shown that the grain shape considerably affects the quasistatic behavior of granular materials [4, 6–9], systematic and quantitative investigations of shape or mixture of shape effects are still elusive. One of the difficulties is that the shape parameters mentioned above need to be defined conveniently in order to be able to generate particle shapes with continuously-variable shape parameters. In addition, particle shape is difficult to control experimentally.

A possible way for studying this problem is to analyze simplified systems with "idealized non-spherical" particles. With this respect, Discrete Element Methods are well suited for this type of simulations even if introducing particle shape in numerical simulations give raise to various technical difficulties such as contact detection and force calculation between particles of arbitrary shape.

Typically, angular shape represents a property of polygonal particles in 2D and polyhedral particles in 3D. Elongation and platyness can be analyzed throughout the aspect ratio parameter. Along the same line, interlocking is a basic feature of non-convex particles and can be represented by aggregate composed of spheres. Thus, the main objective of this work was to analyze numerically the effect of particle shape on the strength properties by varying systematically the shape from spheres to angular, non-convex and elongated/platy shape, as well as by considering mixture of shape.

2 Numerical procedures

2.1 Particle shape parameters

The level of sphericity can be defined by the three ratios $\lambda_1 = L_p/h_p$, $\lambda_2 = l_p/h_p$ and $\lambda_3 = L_p/l_p$, where L_p, l_p and h_p are the principal lengths axis ; see Fig.1(B-c). Consequently, spherical particles are such $\lambda_1 = \lambda_2 = \lambda_3 = 1$, In 2D, elongated particles are modeled as a juxtaposition of two half-disks of radius r and one rectangle of length L and width $2r$ as shown in Fig. 1(B-a). The aspect ratio $\lambda_3 = (L + 2r)/(2r)$ and $\lambda_1 = \lambda_2 = 0$. This particles are named "Rounded-Cap-Rectangle (RCR)". In the same way, in 3D platy particles are modeled as square plates with rounded edges, built as a sphero-polyhedra resulting from sweeping a sphere around a polyhedron. In this case the diagonal of the plate is equal to R and the aspect ratio is given by λ_3.

Non-convex particles are regular aggregates of 4-fold rotational symmetry composed of four overlapping spheres of the same radius r as shown in Fig. 1(B-b). In this case $\lambda_1 = \lambda_2 = \lambda_3 = 1$. This shape can be easily characterized by the ratio $\lambda^* = l/2r$, where l is the distance between the centers of spheres. This parameter varies from 0, corresponding to a sphere, to $\sqrt{3}/2$ corresponding to an aggregate where three coplanar spheres intersect at a single point, so that the radius R of the circumscribing sphere is given by $R = r(1 + \lambda^* \sqrt{3/2})$. Elongated, non-convex and platy shape may also be characterized by their degree of distortion η from a perfectly spherical shape, defined as $\eta = \Delta R/R$, with $\Delta R = R - R'$ and R' the radius of the inscribed circle [10].

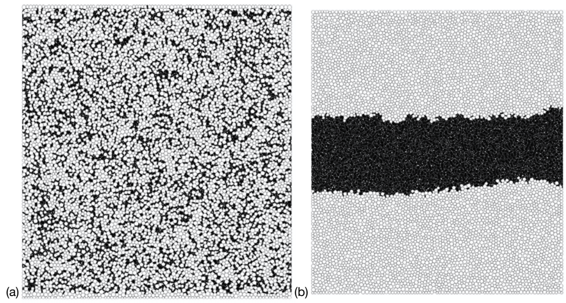

Figure 2. Examples of the generated packings at the initial state, here for binary mixture with $\alpha = 0.5$ and $M^* = 0$ (a) and $M^* = 1$(b). The aspect ratio is fixed at $\eta = 0.7$.

We define the angularity $\langle\alpha\rangle$ of a polyhedral particle as the mean exterior angle between its touching faces. In order to eliminate the effect of particle eccentricity, a strict procedure is implemented in order to isolate and control precisely the shape. First, a set of n_v vertices is randomly generated on a unit sphere. The convex hull of these points is created by associating three vertices for each face. Secondly, we impose that all ratios $\{\lambda_i\}_{i\in 1,3}$ to be greater than 0.9 ; see Fig.1(B-c). This means that, numerically, the sets of vertices are generated until this condition is satisfied. In this simple way, for a given aspect ratio, we can control the angularity of the particles with a single continuously-variable shape parameter depending only to the number of faces n_f.

2.2 Packing construction

We prepared different packings composed of large number of angular or non-convex or platy particles with $n_f \in [596, .., 8]$ or $\eta \in [0, 1[$, respectively. In order to avoid long-range ordering, we introduce a size polydispersity by varying the circumradius R of the particles in the range $[r_{min}, 2r_{min}]$, where r_{min} is the minimum radius with a uniform distribution by volume fractions.

In order to analyse the effect of mixture by particle shape, we built also various packings composed with both discs and rcr particles with $\eta = 0.7$ in 2D. The mixture ratio parameter α is the proportion of elongated particles. We varied α from 0 for a packing composed of only disks to 1 for packing composed of only elongated particles. Mixture homogeneity is measured throughout Lacey mixture indice, which is directly proportional to the standard deviation from a given mean property of one of the constituents of a mixture. Knowing the fully segregated state where all elongated particles belongs in a band of thickness ϵ located at the center of the packing, and homogenous state, the Lacey parameter M^* is given by $M^* = \frac{S_r^2 - S^2}{S_r^2 - S_0^2}$, where S_r and S_0 are the values of the variance of the position of elongated particles calculated from the homogenous and fully segregated systems, respectively. Hence, numerically we constructed various packings with

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M^* varies from 0, for fully segregated system, to 1, for fully homogeneous mixture. Figures 2 displays snapshots of the packings for several values of M^* and α at the end of isotropic compaction (see below).

By means of contact dynamic simulations (CD) [11] the particles are first compacted by isotropic compression inside a box. The gravity is set to 0 as well as friction coefficient μ and μ_w between particles and with the walls. A the end of isotropic compression, the connectivity number, defined as the mean number of contacts per particle (see Sec. 4) is nearly 12 for all packings which is in full agreement with the isostatic nature of our initial packings. These samples are then used as initial configuration for biaxial, respectively triaxial, quasi-static compression tests, for which friction between particles is set to 0.4.

3 Strength properties

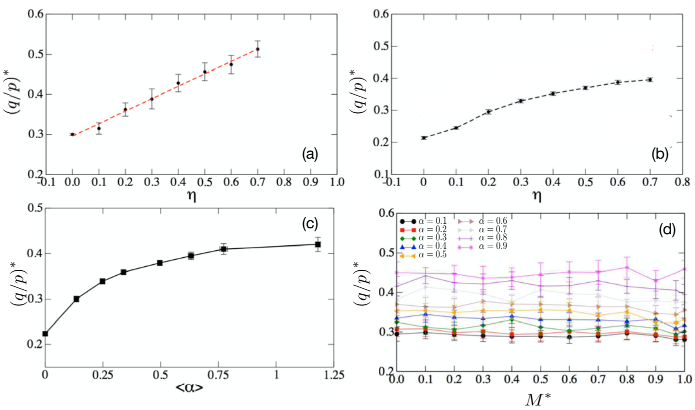

Figure 3. Normalized shear strength averaged in the steady state as a function of particle platyness/elongation (a), non-convexity (b), angularity (c), and as function of packing homogeneity for all values of mixture ratio (d).

In granular systems, the stress tensor σ is given by $\sigma_{\alpha\beta} = n_c \langle f^c_\alpha \ell^c_\beta \rangle_c$, where n_c is the number density of contacts c, $\mathbf{f^c}$ and $\ell^{\mathbf{c}}$ refer to force and branch vector at the contact c, and the average $\langle ... \rangle_c$ runs over all contacts in a control volume [5]. In 3D with axial symmetry we define the stress deviator $q = (\sigma_1 - \sigma_3)/3$ and the mean stress $p = (\sigma_1 + \sigma_2 + \sigma_3)/3$, where $\sigma_{1,2,3}$ are the principal stress values. In 2D, we set $q = (\sigma_1 - \sigma_2)/2$ and $p = (\sigma_1 + \sigma_2)/2$. For our system of perfectly rigid particles, the stress state is characterized by the mean stress p and the normalized shear stress q/p [7]. During shear, the shear stress jumps initially to a high value before decreasing to a nearly constant value in the steady state. The steady-state shear stress $(q/p)^*$ characterizes the shear strength of the material.

Figure 3 shows the evolution of $(q/p)^*$ averaged in the steady state as a function of particle platyness/elongation (a), non-convexity (b), angularity (c), and as function of packing homogeneity for all values of mixture ratio (d). A general observation is that the shear strength increases as shape deviate from spherical shape and also as the proportion of non-spherical particle increases too. But surprisingly, the shear strength saturate at larger values of particles angularity and he remains independent with packing homogeneity. In this last case, this means that homogeneous mixtures have the same strength properties as segregated packings of the two particle shapes.

4 Particle connectivity and origins of strength

The main effect of particle shape is to allow for multiple contacts between particles as shown, for instance, in Fig. 4 for mixture of two shapes and non-convex aggregate. For non-convex particles as those used in this study we can identify seven different types of contacts : 1) "simple" contacts (s), 2) "double-simple" contacts (ds) defined as two simple contacts between two pairs of spheres, 3) " double contacts" (d) defined as two contacts between one sphere of one aggregate and two spheres belonging on the other aggregate, 4) "triple" contacts (t) defined as a combination of simple and double contacts or one sphere of one aggregate and three spheres of another aggregate or three simple contacts, 5) "quadruple" contacts (q) defined as a combination of two double contacts, and 6) five or six contacts with a negligible proportion (below 1%) compared to other contact types. With polyhedral particles, contacts can be grouped in terms of face-face(ff), face-vertex (fv), face-edge (fe) and edge-edge (ee) contacts. With elongated particles we have cap-cap (cc), cap-side (cs) and side-side (ss) contacts. With mixture of two shapes we can consider contact between disks (dd), rcr (rr)and disk-rcr (dr) particles.

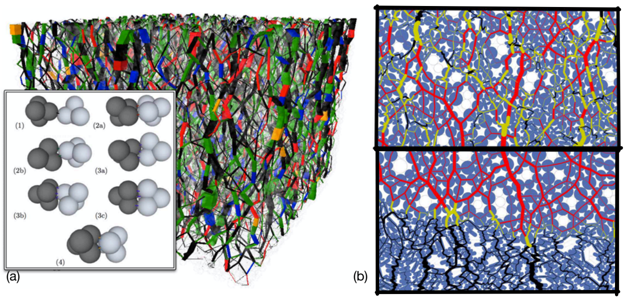

Figure 4. Snapshot of normal forces in (a) packing composed of non-convex particles (here η = 0.6), and (b) packings composed of mixture of two shape for homogeneous (up) and segregated (down) packings. The forces are plotted in different colors depending on contact types. The inset shows contacts type for non-convex aggregate whereas in mixture we can distinguish disks-disks, discs-elongated and elongated-elongated contacts.

To identify the impact of each contact type on the shear strength, we proceed by additive decomposition of the stress tensor according to contact type by $\boldsymbol{\sigma} = \sum_\gamma \boldsymbol{\sigma}_\gamma$, where γ stands alternatively for $\{ff, fv, fe, ee\}$ for polyhedral particles, $\{s, d, sd, t, q\}$ for non-convex particles, $\{cs, cc, cs\}$ for elongated particles and for $\{dd, dr, rr\}$ contacts for mixture of two shapes. The corresponding stress deviators q_γ, are then calculated and normalized by the mean pressure p such $(q/p)^* = \sum_\gamma q_\gamma/p$.

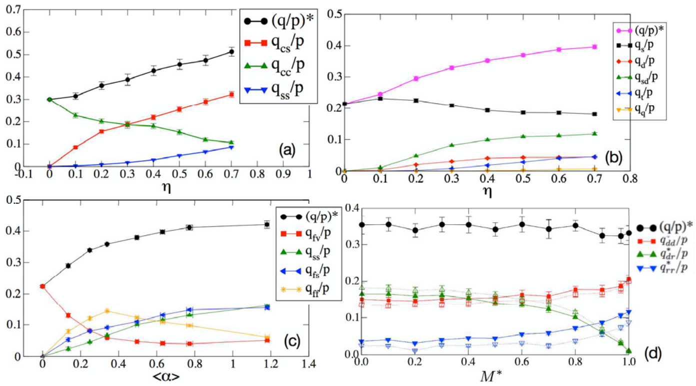

Figure 5. Normalized shear strength as a function of particle shape parameter or Mixing index, for (a) cs, cc and cs contacts in packing composed of elongated particles, (b) s, d, sd, t and q contacts in packing composed of non-convex particles, (c) ff, fv, fe and ee in packing composed of non-convex particles, and (d), dd, dr and rr contacts for mixture of two shapes composed by the same proportion of disk and rcr.

The corresponding normalized stress deviators q_γ/p averaged in the residual state are shown in Fig. 5 as a function of shape parameters, for packings of (a) elongated, (b) non-convex and (c) angular particles, as well as for mixture of two shapes as a function of mixing index M^* for packing composed by the same proportion of disk and rcr. We see that contact types contribute differently on strength properties as function of shapes. For instance, the rapid increase of the shear strength with angularity is due to a rapid increase of strength support by ff contact at low angularity, but the plateau observed for langer angularity is due to a rapid fall off of q_{ff}/p compensated by a rapid increase of q_{fe}/p and q_{fe}/p. For elongated particles $(q/p)^*$ follow q_{cs}/p. And, for mixture of two shapes, we see that q_{dd}/p is nearly constant, whereas remarkably q_{dr}/p follows a trend opposite to that of q_{rr}/p so that the decrease of q_{dr}/p with M^* is exactly compensated by the increase of q_{rr}/p, which explains the independence of $(q/p)^*$ with respect to M^*.

5 Conclusions

In this paper, a systematic numerical analysis of the effect of particle shape properties on the quasistatic rheology of sheared granular media, as well as packings composed of mixtures of two shapes was presented in the framework of Contact Dynamics simulations. The shape of the particles is systematically varied from spherical shape (as referential shape) to angular, non-convex and elongated or platy shape. We considered also binary mixture of disks and elongated particles characterized by the mixture ratio which varies from 0 for a packing composed of only disks to 1 for a packing composed of only rcr particles, and with an homogeneity parameter M^* which varies from 0 for an homogeneous packing to 1 for a fully segregated packing.

A major result of this work is that the particle shape effects are nonlinear and counterintuitive. We show that the shear strength increases as shape deviate from spherical shape. But, for angular shapes it first increases up to a maximum value and then saturates to a constant value as the particles become more angular. For mixture of two shapes, the strength increases with respect of the increase of the proportion of elongated particles, but surprisingly it is independent with the level of homogeneity of the mixture. At the micro-scale we show that various contact types, depending on the specificities of each shape, contribute differently to stress transmission. A general observation is that multiple contact are at the origins of the increase of strength.

In this investigation, the shape was systematically varied along "one" direction. Indeed, we used convex and smooth particles when varying elongation, convex and spherical particles for studying angularity, and spherical and smooth particles for analyzing the effect of non-convexity. However, it should be interesting to vary the shape considering combined effect of elongation and angularity, or elongation and non-convexity, or angularity and non-convexity. In the same way, by analogy with polydisperse packing by particles size, it will be very instructive to consider mixture of various shape, which imply the definition of higher order parameters such particle shape distribution function in order to systematically investigate such effects.

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