Packing of non-spherical aggregate particles by DEM

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Abstract
Loose random and dense random mono-size packing states were investigated by the discrete element modelling (DEM) for eight types of polyhedral grains, for ellipses with different aspect ratio, for cubes and for spheres. Focus was on density, sphericity of the grains and average value and frequency distribution of coordination number. The 3D study was preceded by a 2D one on ellipsoidal disks that offered interesting information, too. Packing has been widely studied in physics and mathematics. Mostly, spherical grains have been considered. However, outcomes of similar studies as discussed herein were recently published in the international literatures. Optimum shape conditions were revealed by our experiments, relevant for optimum aggregate packing in concrete technology. Further, information is obtained on the parameters that reflect packing conditions in an optimum way. The present study involved dense and loose random packing conditions relevant for concrete compacted by vibration and self-consolidating concrete. The cementitious matrix is the major difference with physics test in which generally higher packing densities have been realized. Shape is revealed an important parameter for packing density in all these approaches.

Keywords: Concrete, DEM, packing, aggregate, ellipsoids, polyhedral grains

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Introduction

Packing capacity of aggregate in concrete is obviously of engineering and of economic interest. Although ample research data are available, developments in concrete technology, particularly in the high performance range, ask for additional researches. This can now easier, but still reliably and in a more economical way be performed by DEM. The versatile HADES system is used for that purpose. This is a dynamic concurrent algorithm-based system [1,2]. It renders possible considering arbitrarily shaped particles in packing from the dilute to the dense random state [2]. The particle packing problem is among the oldest in mathematics and physics. So, additional information is available, although mostly dealing with spheres. More recently, also DEM has been employed for packing of ellipsoids [3,4]. The fundamental difference with concrete technology is the matrix. In physics, only hard particles are studied, whereas in concrete technology such grains are surrounded by a cement matrix with a certain consistence. In physics the densest packing is pursued; in concrete technology the gravel grains are embedded in the cementitious matrix that upon hydration binds the aggregate grains together. Packing density is thus inevitably lower than found in such physics studies. Coordination number will be reduced as well.

In our research we have covered spherical particles as well as ellipsoidal ones with various aspect ratios and polyhedral grains of different types. The two categories could represent aggregate of fluvial origin or resulting from a crushing process, respectively. Of course, it is our intention to see whether the aggregate shape will exert similar effects on packing density and coordination number as found in physics. Similarity will allow generalizing the outcomes for optimum aggregate packing purposes, such as in particular for (Super) High Performance Concrete ((S)HPC) and Engineered Cementitious Composites (ECCs). Following a common strategy also in physics studies [3], the 3D study was preceded by a 2D one. In both approaches, shape was varied under loose random packing and dense random packing conditions. The last one will be representative for concrete compacted by vibration, while the first may be closer to the situation pertaining to self-consolidating concrete.

Shape representation of aggregate

The economy of the experiment requires selecting a "representative" shape for a type of aggregate particles, as shown in Fig. 1. For aggregate of fluvial origin, ellipsoidal grains are selected, while for crushed rock aggregate polyhedrons are taken. In both cases, more than one type of grain shape can be selected, of course. A study has focused on the shape analysis of simplified shapes with experimental results by X-ray tomography [5] and simulation strategies has been established for two types of aggregate [6].

Figure 1: Representation of river gravel and crushed rock aggregates by ellipsoids and polyhedrons, respectively
Structure generation

The HADES system is a dynamic concurrent algorithm-based DEM. Particle interference is an integral part of DEM; in a dynamic system this is accomplished by having the particles "moving around". The procedure is such that the grain mixture in which the particles have a desired shape is dilute dispersed in a container. Hence, in this stage a random sequential addition (RSA) system can be of profitable use. For generation of the densely packed aggregate structure, such systems yield a biased solution, despite being quite popular in concrete technology [7]. Next, grains are provided with a thin guard zone and are set to move according to a Newtonian system for linear and rotational motion. Surfaces of the grains are tessellated into a triangular system. Upon overlap of guard zones of colliding grains, interaction forces between the associated tessellated surface elements develop. This force is a function of distances and areas of the segments and is integrated for the activated part of the surface. Such forces can be spring-like, leading to repulsion, cohesive, leading to attraction, or represent damping (due to energy losses in the system) and friction effects.

The grains also similarly interact with the mould of the container, whereby the container boundaries can be periodic, rigid, or a combination. During this dynamic stage, the container is shrinking in size until the desired volume fraction is attained of the grains, in the present case representing an aggregate mixture. The guard zones lead to small boundary gaps between the grains (Fig. 2). This has been at least partly compensated for by a growth process of the grains. Maximum packing density could have been obtained by application of randomized shifts and rotations in places where overlap is found. However, in concrete technology this would be an irrelevant action, because of the presence of the cement matrix. Examples of random loose packed crushed rock aggregate structures represented by polyhedrons subjected to growth are shown in Figs. 3 and 4.

Figure 2: Growth for eliminating gap by guard zone in HADES simulation

Figure 3: Packed structures of arbitrary octahedrons with rough surface texture at different growth levels, respectively 0.1, 0.2, 0.3 and 0.4 mm
In physics experiments similar structure generation procedures pertain. Ref. [4] may serve as an example. Authors generate ellipses by a RSA (random generator-based) procedure and discretize the perimeter, so that polygons are resulting. Thereupon growth is step-wise applied. Whereas in our research we stop when overlap is exceeding a certain limit, in this physics experiments they locally shift and rotate the polygons for elimination of overlap. These growth steps are applied until total overlap is also exceeding a minim level. This is in fact the procedure of a static DEM.

**Effect of grain shape on packing**

In the 2D physics experiments on multi-size ellipses in the “jammed state”, authors in [8] find the volume density of 0.84 for circles to increase with aspect ratio \( \lambda \) to a value of about 0.9 for \( \lambda \sim 0.7 \), whereupon it declines again. For \( \lambda < 0.25 \) the packing density is even below that of the circles. At the proper sensitivity level for the assessment of contacts between ellipses, the average contact number increases from 4 for circles to a plateau value of 5.7 reached at \( \lambda \sim 0.6 \) (6 being the theoretical value for the average number of contacts of jammed ellipses).

Donev *et al.* [3] presented data in 3D on mono-size ellipsoids and spheroids obtained by a dynamic concurrent algorithm-based DEM. In both cases, the volume fraction at random dense packing of spheres of 0.64 increases to 0.71 for spheroids at an aspect ratio of about 0.6, and for ellipsoids to only a slightly higher volume fraction at an aspect ratio of about 1.5. Average number of contacts per particle increased in both cases from about 6 to 10, approximately. All those simulations use periodic boundaries for exclusion of wall effects. Comparison with experiments in real containers (like those with M&Ms Milk Chocolate Candies) is therefore not straightforward.

In our simulation we also employed periodic boundaries. Fig. 5 presents simulations in 2D of ellipses in loose random packing state at different elongations (reciprocal of aspect ratio). Fig. 6 gives the same mixtures but compressed from the top to higher density. Fig. 7 shows the density differences for both regimes at different elongation. The curve for compacted grains is quite similar to that in [8] on a slightly lower level. Average coordination number of circles is about 4, however it is lower than in [8] for the ellipses. This is due to different algorithms as well as different particle samples being used. Delaney *et al.* [3] used a poly-disperse particle size distribution to avoid the ordered structure, which can obviously increase the coordination number.

A similar procedure is followed in the case of the 3D packing of mono-sized standard polyhedrons (with facet number 4 to 8) and a irregularly-shaped particle. 864 particles with sieve size 10 mm were used for each simulation. Fig. 8 visually illustrates some loose packed structures with several typical shapes. As facet number and sphericity are the
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Figure 5: Loose packed structures of mono-sized ellipses for different elongation values

Figure 6: Dense random structures of mono-size ellipses for different elongation values

Figure 7: Packing density of Figs. 5 and 6 as a function of elongation (left) and frequency distribution of coordination number

Sensitive parameter for these shapes, loose packing density is presented in Fig. 9 as function of these parameters. Sphericity is defined as the surface area ratio of equivalent sphere with particle (both having equal volume). Loose random packing density is generally increased with increasing facet number and sphericity as similarly found in case of random dense packing [9]. Both cases of
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packing density have revealed particle shape as an extremely important factor in particle packing. It seems that polyhedrons with larger sphericity can be packed to higher density. Dense random packing simulations with compaction have also been performed based on the aforementioned particle generation strategy. 216 mono-sized particles (d=10 mm) have been used for each packing model. No gravity is involved. Fig. 10 visually illustrates some packing structures of differently shaped grains. As sphericity is a sensitive parameter in these ten shapes (nine faceted polyhedra plus sphere), the relationship of sphericity and maximum packing density is shown in Fig. 11. Dense random packing density of tetrahedrons and cubes complies with findings in [9].

Figure 8: Mono-size random loose packing states of particles with some typical shapes

Figure 9: Random loose packing density as function of (left) facet number and (right) sphericity of particles shown in Fig. 10.

Figure 10: Mono-sized random packing with particles having typical shapes: (a) tetrahedron (b) hexahedron (c) octahedron and (d) sphere, respectively.
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Figure 11: Dependency of maximum packing density on (left) facet number and (right) sphericity of 3D particles shown in Fig. 10.

Coordination number is an important parameter for evaluating packing efficiency. Similar as in 2D space, a numerical method is established for calculation of coordination number of a packed system of arbitrary-shaped particles. Certain additional mesh and evaluation points are applied to surface of particles for the assessment purpose. Its precision is related to the fineness of the evaluation mesh. Selecting a coarse mesh speeds up the calculation, but leads to biased results. Therefore, a refined mesh should be applied for the calculation of coordination number.

This method has been applied for the evaluation of coordination numbers in the random dense packed structures of Fig. 10. The distributions of coordination number with different shapes are presented in Fig. 12. Coordination numbers in polyhedron packing are also not only related to packing density, but also related to shape. For instance, average coordination number of ordered packing of cubes is only 6, while packing density can reach to 1.0.

Figure 12: Frequency distributions of coordination number of dense packed polyhedrons of different types
Conclusions

Effect of grain shape on packing was found fundamentally similar as in physics simulations and experiments. Coordination numbers were somewhat reduced because of using different algorithms. Differences are irrelevant because cement matrix will reduce coordination numbers in concrete. For river aggregate we see that non-spherical grains can lead to improved density which will exert positive effects on strength and durability as well as on economy. For crushed rock we see an increase in packing density with sphericity and facet number. Whether this can be exploited in future is uncertain, of course, but it may be an interesting aspect in the design of super high performance concretes, of course. DEM has proven a economic and reliable tool for investigating effect of technological parameters on packing and can as a consequence play a major role in studies on mechanical [10] and durability [11] properties.

References