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Particle shape and its importance to Discrete Element Modeling in the context of railway ballast simulation

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Abstract. Computational tools may be helpful to understand the railway ballast mechanical behavior. In the context of the Discrete Element Method (DEM), a numerical simulation may be performed considering different grain shapes and parameters to represent the actual ballast. It is well-known that modeling faceted aggregates (polyhedral) provides interlocking between particles. This may avoid rolling movements. On the other hand, employing spherical particles to represent non-spherical grains may neglect the physical expected rolling resistance. In this paper a shear box test simulation using DEM was investigated, considering distinct shapes of ballast aggregate. The macroscopic mechanical behavior will be addressed for each case. It will be considered realist railway ballast retained at sieves of 25 mm, 38 mm and 50 mm. An inexpensive laser scanning technique is also employed with realistic grains, in order to incorporate their shape into the DEM. An extensive parametric study was conducted exploring the influence of the particle shape (spheres, basic polyhedral and scanned particles), in order to find the best compromise way to simulate a desirable scenario, from the engineering point of view.

Keywords: discrete element method, ballast, shape, direct shear test.

1 Introduction

The ballast is a free draining granular material that consists of strong angular particles, as defined by Indraratna and Ngo [1]. Most of its grains varies in size from 25 mm to 63 mm, according to ABNT NBR 5564 [2]. Its importance stems from the fact that it is a structural support layer and its shear strength is crucial to the railway lateral resistance. Furthermore, it has to provide rail alignment and conformity to the railway design characteristics, such as superelevation. Due to that, it requires periodic maintenance.

In order to simulate its global behavior, it is essential to analyze each particle interaction individually. For this reason, the discrete element method (DEM), introduced by Cundall and Strack [3] in 1979, was selected. This method was, initially, developed for spheres due to their simplicity, making it easier and faster to calculate the particle-particle and particle-boundary contacts by applying Newton's second law of motion. However, the majority ballast grain shapes are not spherical.

This correlation between spheres and other shapes can be seen by the sphericity parameter. It varies from almost zero to one, when the particle is a perfect sphere. This description was first introduced by Wadell [4] in 1932, and had many definitions through time. In 2004, it was modified by Santamarina and Cho [5], in order to make it independent of the surface area and, consequently, the roughness of the material. It was then defined as the ratio of the maximum inscribed sphere diameter to the minimum circumscribed one.

Another important parameter used to characterize a grain shape is the aspect ratio (AR). This analysis, according to ABNT NBR 5564 [2], consists in measuring 3 perpendicular specific dimensions, in order to determine the horizontal (HAR) and vertical aspect ratios (VAR) for each particle. Then, based on the AR, it is possible to classify them as: cubic, elongated, flat and flat-elongated. Cleary and Sawley [6], when studying particle shape influence on a hopper discharge with DEM, concluded that elongated particles had a decrease of the flow rate of 30% when compared to the circular particles. Another study about the particles shape, developed by Höhner, Wirtz and Scherer [7], showed that an increase in the aspect ratio resulted in an enhancement of apparent shear strength.

According to Zhao, Zhou and Liu [8], higher angularity increases the particle-particle interlocking, so polyhedral particles tend to have a strong interlocking when compared to spherical particles. This effect provides a more realistic load-deformation response, as reported by Lu and McDowell [9]. Usually, the angularity is inversely proportional to the number of faces/vertices and the interlocking effect enhances the shear resistance.

Several techniques have been developed in order to capture the different aspects of particles geometry. Some of these methods are: laser scanning [10], photogrammetry [11] and computerized tomography [12]. These captured geometries can be inserted into a DEM software with some simplifications, in order to make it viable in terms of computational cost usually as a cluster of spheres or a custom polyhedron with reduced number of faces. Another simplification that can be done is a shape transformation from concave to convex.

Rocky DEM [13] is the commercial DEM software chosen to conduct this paper analysis. In addition to spheres, it allows the use of polyhedra that can be created by inserting some geometric parameters or custom polyhedra that can be introduced by a STL file with the most desirable shape. This type of geometry will be addressed as “scanned particle”, because the imported shape came from the scanning process.

This paper approach is focused on comparing spherical, polyhedral and scanned particles, showing their behavior when subjected to a shear box test. Moreover, analyzing the simplification process interference on the scanned grains properties. Finally, likening polyhedral particles with different aspect ratios and proposing an alternative to the scanning process based on it.

2 Methodology

2.1 Ballast shape

In this study, a ballast sample was collected and subjected to a granulometry and shape tests according to ABNT NBR NM 248 [14] and ABNT NBR 5564 [2], respectively. The scanning process was conducted only for particles retained at sieves with mass retention superior to 10%. As a consequence, the shape analysis was executed within this condition. For this reason, the particles retained at the sieves of 25 mm, 38 mm and 50 mm were studied, which represent 93% of the total sample mass examined.

The shape analysis was conducted manually with a pachymeter for a total of 94 particles chosen proportionally to the retained amount at these sieves. This analysis consists in measuring 3 specific particle dimensions that are equivalent to inscribing the grain by a parallelogram with its largest side parallel to the largest particle dimension. Naming a, b and c the sides of this parallelogram in a decrescent order, the horizontal aspect ratio (HAR) is defined by b/a and the vertical aspect ratio (VAR) by c/b.

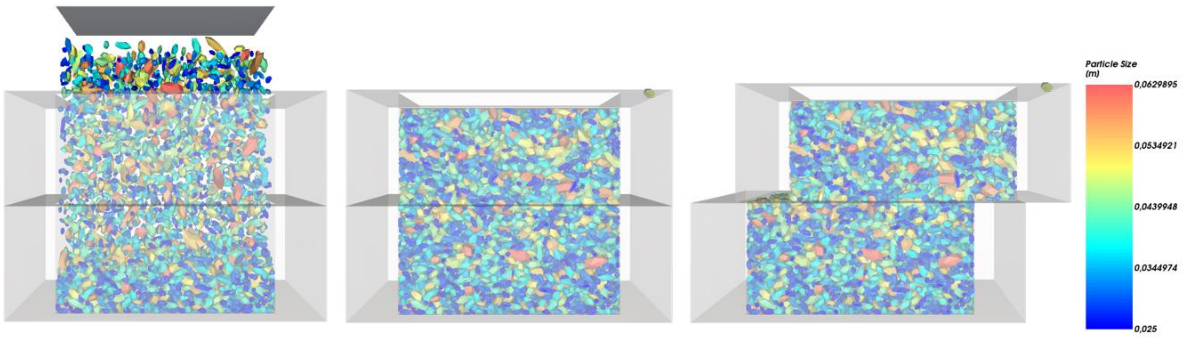
From this sample, 90 particles were selected to be scanned, proportionally, to the amount of grains retained at each of these sieves. For this purpose, the BQ Ciclop was chosen as an inexpensive laser scanner designed with a rotation platform that allows a 360 degrees scanning. It creates a point cloud that requires some manual interference to treat undesirable captured points. This data was processed by MeshLab [15] with the “Screened Poisson Surface Reconstruction” algorithm that results in a surface with, approximately, 150,000 faces. This number is considered large to be handled by DEM, thus it was reduced to 50 and 24 faces and then transformed to a perfect convex particle by the Rocky’s algorithm, in order to make the DEM simulation viable. The shape analysis was also conducted at the scanned particles, along with calculations of a sphericity and volumetry.

A polyhedral particle in Rocky DEM [13] software can be created by inserting, among other parameters, the number of faces, the sieve size and the horizontal and vertical aspect ratio. Thus, a script was developed to create a set of 24-face particles with the same aspect ratios as the scanned ones, this method was named Equivalent Aspect Ratios (Equivalent ARs).

2.2 Direct shear test

The direct shear test is a popular and relatively simple procedure capable of measuring shear stress, strength and displacement, according to Po-kai, Kenichi and Fumio [16]. Particles, with no cohesion, are inserted into a split box (Figure 1a) in a loosen state. Then, a vertical force is applied upon all grains distributed by a plate (Figure 1b), making the whole specimen to experience a given normal stress state, that in this case was defined as 196 kPa. Next, a lateral horizontal displacement is inflicted at the bottom half of the box (Figure 1c), with a continuum speed of 0.01 m/s. The force required for this displacement is measured and, as the shear plane is known, it is possible to calculate the shear stress as a function of the lateral displacement. This relation between stress and strain leads to the so-called "stress curves".

The highest stress value obtained is named "peak shear stress" and the stress at the end of the experiment, for a horizontal displacement of 180 mm, is the "residual shear stress". It is known that the compaction of the ballast influences significantly the peak shear stress whilst does not change the residual one [17]. Higher apparent density levels increase the peak shear stress, while the peak and residual shear stresses are similar for more loosen particles.



(a) (b) (c)

Figure 1. Shear box setup: (a) inserting particles, (b) applying vertical top force and (c) prescribing a horizontal displacement

The input simulation parameters are specified in Table 1. Moreover, the normal and tangential force models chosen are the Hertzian Spring-Dashpot and the Linear Spring Coulomb Limit, respectively. The shear box simulated is considered large (1 m³), in order to be able to simulate ballast particles without the boundary interference. The shear box was modeled based on the experiment developed by Estaire and Santana [17], which dimensions allow the study of particles with up to 85 mm diameter.

Table 1. Input simulation parameters

Category	Input Parameter	Value	Category	Input Parameter	Value
Particle properties	Density	27 kN/m³	Boundary properties	Density	27 kN/m³
	Young's modulus	0.25 GPa		Young's Modulus	0.25 GPa
	Poisson ratio	0.20		Poisson ratio	0.20
Particle-particle contact properties	Static friction	0.90	Particle-boundary contact properties	Static friction	0.43
	Dynamic friction	0.80		Dynamic friction	0.34
	Tangential stiffness ratio	1.00		Tangential stiffness ratio	0.80
	Restitution coefficient	0.10		Restitution coefficient	0.30

It is worth mentioning that by running the same simulation twice, it is possible to notice a minor dissimilarity between them. This occurs because the particles are generated randomly, therefore the specimen configuration will be different each time, resulting in slightly distinct outcomes.

3 Results

3.1 Scanned particle shape analysis

The scanned particles and the simplification processes were analyzed. It can be seen (Table 2) that reducing the number of faces decreases significantly the volume (15.7%), area (10.8%) and sphericity (9.9%) of the particles, when comparing the concave simplified to 1000-face particles to the concave more simplified ones, with 24 faces. On the contrary, the concave to convex transformation caused an increase in volume: 7.7% on 24-face particles and 25.9% on the 50-face ones. Furthermore, no significant changes on the aspect ratios were noticed. However, the original particles analyzed manually by the procedure on ABNT NBR 5564 [2] presented an average horizontal and vertical aspect ratio of 0.71 and 0.60, respectively; what suggests a size increment from the scanning process, when compared to the 1000-face concave particle (HAR 0.76 and VAR 0.65). Although the scanning error is an important aspect, this paper focus on the propagation of error by the simplification process.

Table 2. Average properties of the simplified particles

Average properties	Concave 1000 faces	Concave 50 faces	Concave 24 faces	Convex 50 faces	Convex 24 faces
Volume (mm³)	34212.6	29683.6	28825.8	37370.8	31033.5
Área (mm²)	6414.5	5832.8	5723.5	6322.2	5763.3
Sphericity	0.395	0.377	0.356	0.379	0.356
Horizontal Aspect Ratio	0.76	0.76	0.75	0.75	0.75
Vertical Aspect Ratio	0.65	0.63	0.63	0.64	0.63

It is noticeable, from Figure 2, that the surface texture information was lost in this process, but the general shape was kept. In addition, it is apparent that the transformation from concave to convex shape was subtle and did not change any unnecessary boundary, maintaining the overall aspect ratios and sphericity.

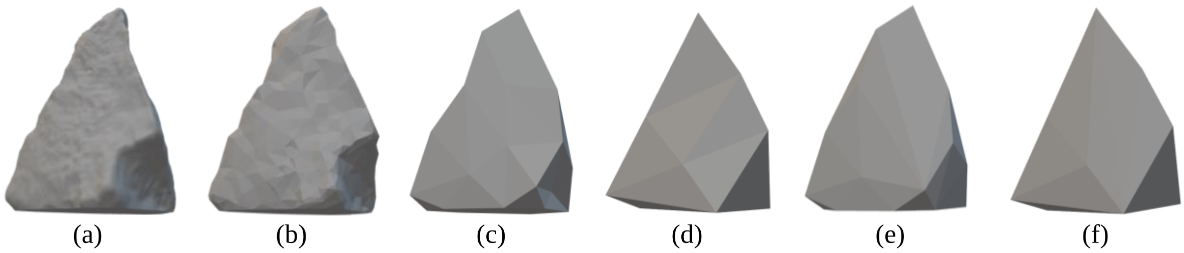
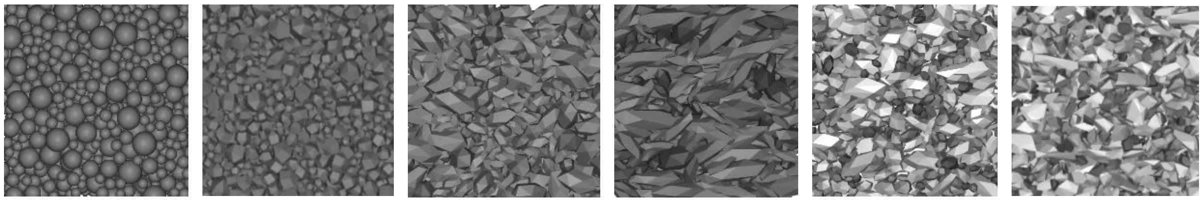


Figure 2. Scanned particles of (a) concave 150.000 faces, (b) concave 1000 faces, (c) concave 50 faces, (d) concave 24 faces, (e) convex 50 faces and (f) convex 24 faces

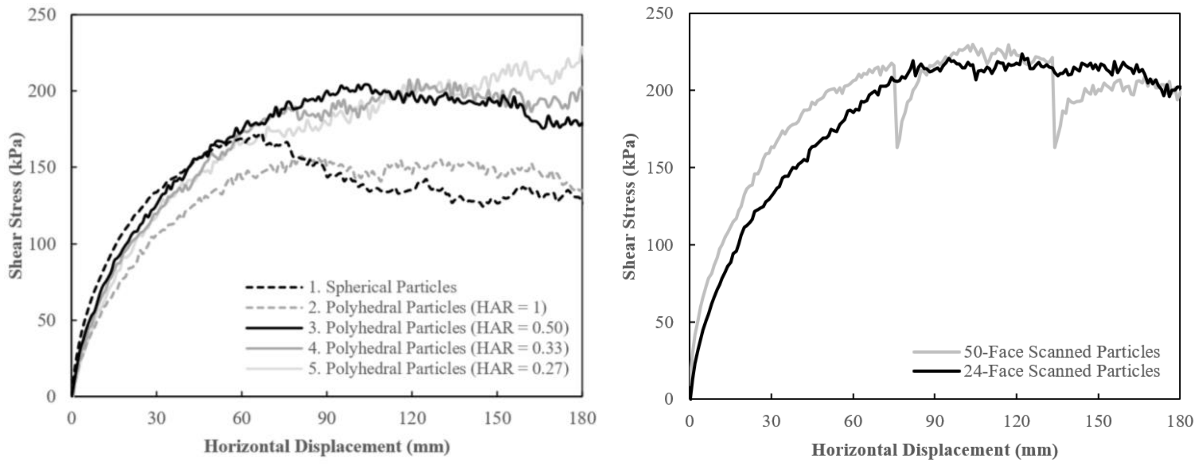
3.2 Direct shear tests

Different concave particle shapes were analyzed (Fig. 3) in the context of their shear stress when subjected to a shear box test. It can be seen, from Fig. 4a, that the aspect ratio is one of the key geometric factors that influence the shear behavior on grains. Altering just the horizontal aspect ratio, from 1 to 0.50, resulted in an increase of the peak shear stress of 30%. This modification had a serious impact on the sphericity of the particles, decreasing it from 0.75 to 0.42, a total of 44% reduction. Additionally, the average flip count, that is the number of times a particle rotates around itself, decreased 24%. Thus, that indicates a strong correlation between sphericity, aspect ratio, rolling behavior and shear stresses. This is one of the reasons why spheres present lower shear stress values when compared to the polyhedral grains and, usually, require the artificial parameter called “rolling resistance”, in order to impose a non-existing geometric attribute to the spherical shape particle. This artificial parameter was not considered in this paper.



(a) (b) (c) (d) (e) (f)

Figure 3. Particle shapes: (a) spheres, polyhedra of (b) 1 HAR, (c) 0.5 HAR, (d) 0.27 HAR, (e) equivalent ARs and (f) 24-face scanned particles



(a) (b)

Figure 4. Shear stress vs horizontal displacement for (a) spherical and polyhedral particles with different aspect ratios and (b) the scanned particles of 24 and 50 faces

Table 3. Apparent density, peak and residual shear stresses of the Fig. 4a particles

Type	**Peak Shear Stress (kPa)**	**Residual Shear Stress (kPa)**	**Apparent Density (kN/m³)**
1. Spherical Particles	173	127	17.67
2. Polyhedral Particles (HAR = 1)	157	135	17.12
3. Polyhedral Particles (HAR = 0.50)	204	179	17.11
4. Polyhedral Particles (HAR = 0.33)	207	202	16.27
5. Polyhedral Particles (HAR = 0.27)	229	229	15.74

It may be observed, from Tab. 3, that the geometric properties of the particles influence the compaction level. The rearrangement of the grains for different aspect ratios implied an apparent density variation that is directly associated with the behavior of the curves. The spherical particles showed the highest variation between the peak and residual shear stresses and the highest density, while the polyhedral particles with HAR of 0.27 displayed no variation and the smaller density among all the particles studied in Fig. 4a.

The comparison between the scanned particles of 24 and 50 faces (Fig. 4b) shows a good correlation and the difference on their peak and residual shear stresses values are not larger than 7% and 1.5%, respectively. Although, the 50 faces particles display a higher initial stiffness. These two steep drops observed at the scanned 50 faces particles are described, by Liu, Gau and Chen [12], as the breakage of a strong contact that is replaced gradually by the development of a new one.

Indeed, it is noticeable that the aspect ratio plays a significant role to the shear strength of the aggregates. Based on this, in order to mimic the results obtained from the convex 24 faces scanned polyhedron, without the need of the scanning process, two numerical experiments were done (Figure 5). The first one, denominated Average ARs, tries to reproduce the results using only one type of particle employing the sample average aspect ratios (0.75 HAR and 0.63 VAR). This simulation resulted in a 14% decrease of the peak and residual shear stresses. When analyzing the distribution of the aspect ratios (Figure 6), it is possible to see a distribution with large standard deviations, thus, a more disperse AR distribution.

The second experiment, named Equivalent ARs, which consisted in creating a set of 90 polyhedra particles with the same aspect ratios of each scanned grain from the sample, was conducted. The outcome for this simulation is very similar to the scanned simplified 24 faces sample and their difference peak and residual shear stresses obtained are inferior than 5.5% and 2.5%, respectively. It can be seen, from Figure 6, that the aspect ratio distribution among particles is slightly different, when comparing the scanned to the Equivalent ARs particles, especially for the HAR. One of the reasons for that is a software limitation that does not allow HAR smaller than 0.50.

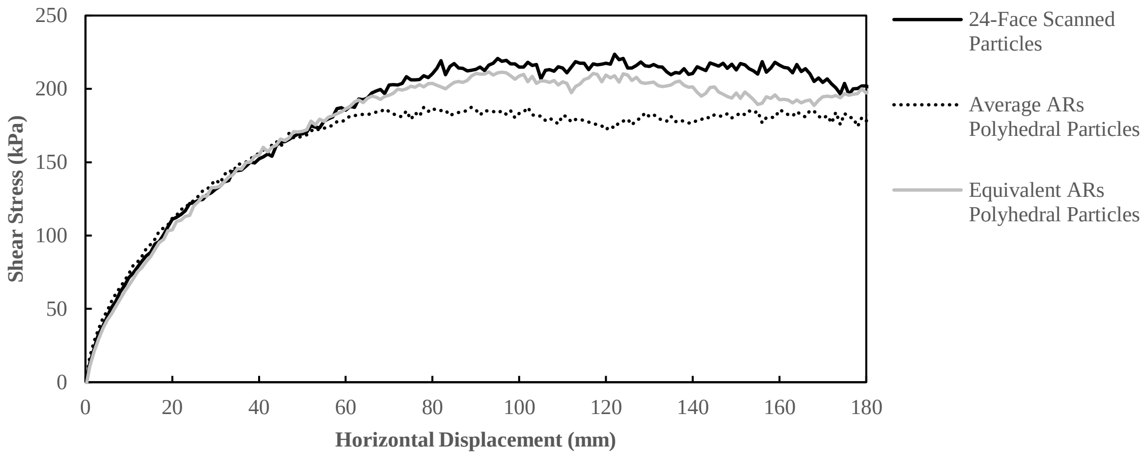
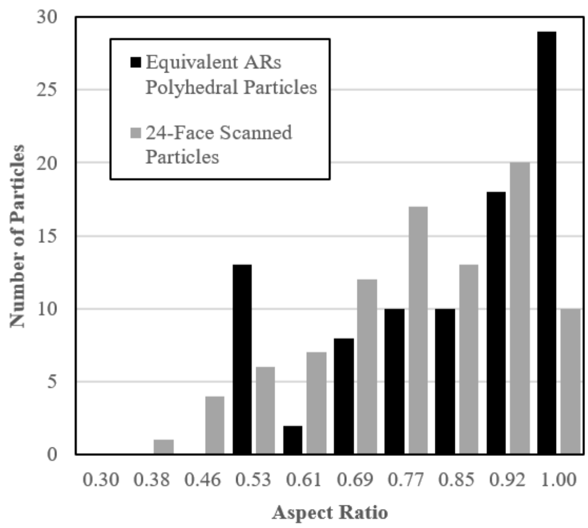
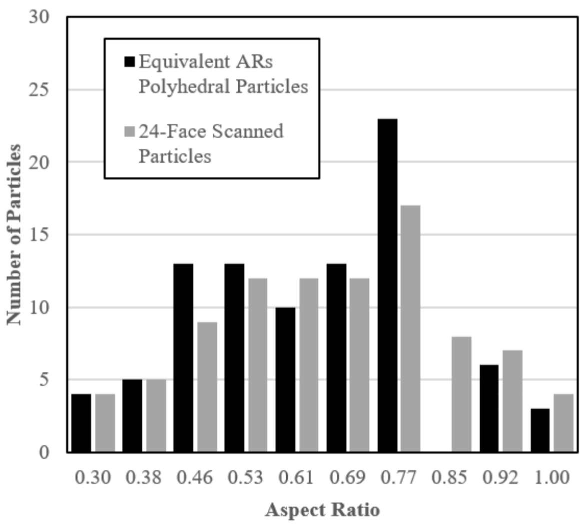


Figure 5. Shear stress vs horizontal displacement for the scanned particles and average and equivalent ARs polyhedron particles



(a)



(b)

Figure 6. Histograms comparing the Equivalent ARs particles and the 24-face scanned ones by (a) the HAR and (b) the VAR

4 Conclusions

This paper analyzes the influence of the particle geometry on the overall mechanical behavior of a box full of particles experiencing shearing (shear test). Spheres, polyhedra and scanned polyhedra grains were studied. The shape of the particles showed to have a direct link to the shear stress resistance. The aspect ratio of particles showed to be a crucial parameter, in the context. Altering the aspect ratio changes the rearrangement of the particles. As a consequence, it affects the interlocking and the apparent density of the specimen. Moreover, spheres struggle to represent non-spherical particles without the artificial rolling resistance coefficient. Actual particles do have rolling resistance, due to their shape, affecting the overall shear strength of the particle pack.

The increment on the number of faces considered in polyhedral modeling from 24 to 50 did not show significant changes when analyzing the peak and residual stress points. However, the initial shear stiffness behavior has been altered. Although, further studies are necessary to fully understand this correlation.

The scanning process of particles may require a series of simplifications that result in considerable changes of geometric parameters. Thus, obtaining just the aspect ratios from a particle sample, according to the ABNT NBR 5564 [2] shape analysis, is enough to represent almost the same shear behavior of the simplified scanned particles; without the need for a time demanding scanning process.

The conclusions here were done in the context of a shear box text. However, the applications motivating such a study come from railway engineering. In this context, a deep understanding of the mechanical behavior of the railway ballast (particularly when experiencing shear) is essential to understand the performance and stability of the railway track.

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