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Porosity of random granular media of monosized polyhedra

Jesús, Sánchez Guzmán
Facultad de Estudios Superiores Aragón, UNAM, México, México, jesusguzmane2@aragon.unam.mx

Gabriel Auvinet
Instituto de Ingeniería, UNAM, México

ABSTRACT: For geotechnics and other areas, the study of granular materials constituted of non-spherical particles is of interest. In this paper, an analysis of the porosity of granular materials of identical grains in the shape of polyhedra is presented: tetrahedra, cubes, octahedra, dodecahedra, icosahedra, square plates, regular quadrangular prisms, and spheres. Each polyhedron is formed by a clump of spheres of different sizes. Resorting to Discrete Element Method, granular samples are constructed by gravity and brought to static equilibrium. The inherent porosity of each sample is then evaluated by the Monte Carlo technique. It is observed that the geometry of the particles significantly affects the porosity of a granular medium. The results indicate that the granular material with spherical grains is the least porous. The granular sample of tetrahedra presents the maximum porosity among regular polyhedra. In materials formed by plates or prisms, the minimum porosity corresponds to the sample of cubes. On the contrary, the porosity of the medium increases when its particles present a very different dimension with respect to the other two. The results obtained show trends in the effect of the grains geometry on the porosity of random granular media. Different sources of error in the study are identified.

KEYWORDS: porosity, granular media, clump of spheres, polyhedra, geometry of grains.

1 INTRODUCTION

In the studies of granular media, spherical particles are usually employed, because they present the most elementary geometric shape and allow different concepts to be formally introduced. However, in areas such as geotechnics, soil grains are irregular and in the analysis of their characteristics, especially porosity, it is necessary to consider the geometry of the particles.

Studying the void space of a granular material is a formidable task, even for the most basic cases (Hales, 2005). The study of porosity in regular and random arrangements of spherical particles has been the subject of various works such as Caquot (1937), Auvinet (1986), Dias *et al*. (2004), Sánchez *et al*. (2015) and others.

An important step towards greater realism is to represent grains with other geometric shapes that are ubiquitous in nature (Zenil, 2011), the polyhedra. This is a topic open to investigation because currently various studies in geomechanics are being carried out with highly idealized geometries (Tran *et al*., 2025; Zheng *et al*., 2025).

The objective of this work is precisely to study the porosity of granular materials constituted by regular polyhedra. Only the case of random arrangements of identical particles is explored. The analysis is performed using numerical simulations resorting to the Discrete Element Method (DEM) and probability and statistics theory.

2 SOILS POROSITY

The study of the volume of voids in a soil, parameters such as porosity, void ratio and relative density are used. Porosity is defined as the fraction of the total volume of a medium occupied by voids; It stands out as the most stable parameter (Auvinet, 2019) among those mentioned and the one that lends itself best to statistical analysis.

The porosity of a granular medium depends on different factors such as: grain size distribution (Furnas, 1931, Caquot, 1937, Marsal, 1977, Auvinet, 1986, Auvinet and Bouvard, 1987, Mota *et al*., 2001, Dias *et al*., 2004, and Browers, 2011), sample formation methods (Zhang *et al*., 2001; Sánchez *et al*., 2015), friction on the surface of the grains (Sánchez, 2017) and particle geometry (Teich *et al*., 2016).

The porosity of soils can vary in a wide range. Typical observed values are 0.2 for well-graded soils, 0.4 for sand or gravel (Liu *et al*., 2019), and 0.7 for soils with flattened particles (Jackson *et al*., 1978).

Theoretical studies, physical tests and numerical simulations, frequently resort to a spherical representation of the particles. For arrangements of spheres of equal size (monosized), the minimum porosity is 0.26 according to the Kepler Conjecture (Hales, 2005), the maximum is 0.48 for regular assemblies, and 0.44 for random ones (Caquot, 1937). Binary mixtures (spheres of two sizes) are less porous due to components interaction (Furnas, 1931, Bezrukov *et al*., 2001; Sánchez *et al*., 2015). Materials of three or more components and with continuous grain size distribution, generally present intermediate porosities (Auvinet, 1986, Sánchez, 2017, Auvinet and Sánchez, 2023).

For granular media made up of polyhedra, the porosity can vary more than in the case of spherical particles. For example, with regular and semi-regular polyhedra, the three-dimensional space can be filled and lead to zero porosity (Viana, 2018). The maximum values are unknown.

3 NUMERICAL ESTIMATION OF POROSITY

In a granular arrangement of spherical particles, it is possible to calculate the exact volume of the solids, V_s, contained in an analysis region with volume V_T and obtain the porosity as $n = 1 - V_S / V_T$. However, this procedure can be cumbersome for complex geometry and intersections between grains.

Another alternative to estimating the porosity is the Monte Carlo technique. In this method, N points are generated randomly in space and the number of points that fall into the voids (N_V) is counted. The quotient N_V/N converges in probability towards porosity. Considering that N_V is a random variable with a binomial distribution, the standard deviation (σ) of the estimated porosity is given by Equation (1) (Auvinet and Bouvard, 1983).

$$\sigma = \sqrt{\frac{n(1-n)}{N}} \tag{1}$$

In what follows, the Monte Carlo technique is used to estimate the porosity. If *a priori* n=0.4 and N=10^6 are proposed, it is obtained σ=0.0005, and it is accepted as a negligible error.

4 SIMULATION OF GRANULAR SAMPLES

4.1 *Geometric representation of the grains*

In most numerical models of granular media, the elementary form to represent particles is the sphere. To reproduce other geometric shapes, different techniques can be used (Cundall, 1971, Wang, 2007; García *et al*., 1009; Gao *et al*., 2012). In this work, the algorithm of Taghavi (2011) implemented in PFC v5 (Itasca, 2016) is used. This algorithm fills a volume with a set of spheres secant to each other and tangent to the boundary surface. The solid body is approximated by a clump with a quality that depends on the ratio $\rho = D_2/D_1$ and the angle of intersection, φ, between spheres (Figure 1). D_1 and D_2 can vary from a minimum diameter D_{min} to maximum one D_{max}.

The Monte Carlo technique can also be used to evaluate the quality of the representation of a polyhedron. Taking the cube of the Figure 1 a) as an example, values of ρ and φ are proposed. For each pair of values, a clump is constructed and the ratio Vg/Vc is obtained, which represents the volume of the clump, Vg, with respect to the volume of the cube, Vc.

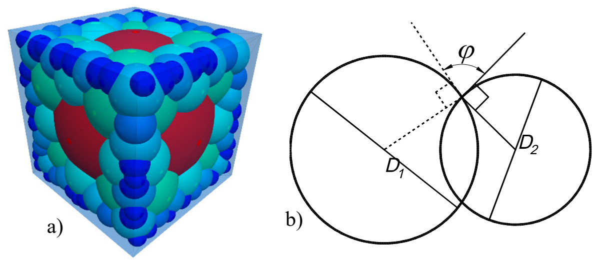

Figure 1. Approximation of a polyhedron: a) clump of spheres and b) intersection between he spheres on the clump

Figure 2 presents the variation of Vg/Vc and the number of spheres, Ne, used in the representation of a cube. For constant φ and $\rho \in [0.05, 0.2]$, starting from the upper limit of the interval, it is observed that 86% of the volume of the cube is filled with 52 spheres. Figure 2 a) shows that approximation improves as ρ decreases, but the number of spheres increases dramatically to keep $\varphi = 120°$ constant. For $\rho < 0.1$, no major improvements are obtained.

In the other hand, adopting the value $\rho = 0.1$ as constant and varying φ in the interval [100, 150°], Figure 2 b) Vg/Vc increases approximately linearly until reaching values close to 1. This is accompanied by an exponential increase in the number of spheres employed.

In section 4.2, some granular samples of identical cubes were created with the procedure described below. In each case, a different quality, Vg/Vc, is used in the representation of the cubes and it is observed that the porosity of the medium increases when the Vg/Vc ratio increases. This is explained by the fact that the sharpest vertices of the cubes open the granular structure.

Considering the available computational capacity, that porosity varies less than 1% when the representation of the cubes is improved, and that the grains of geotechnical materials are not perfect polyhedra, $\rho = 0.1$ and $\varphi = 120°$ are adopted to represent the grains of the present study.

As noted earlier, most numerical simulations of granular media assume spherical particle shapes. However, the geometry of soil grains is irregular and complex to simulate. Therefore, an intermediate step in the study of granular media involves representing the particles by means of regular polyhedra.

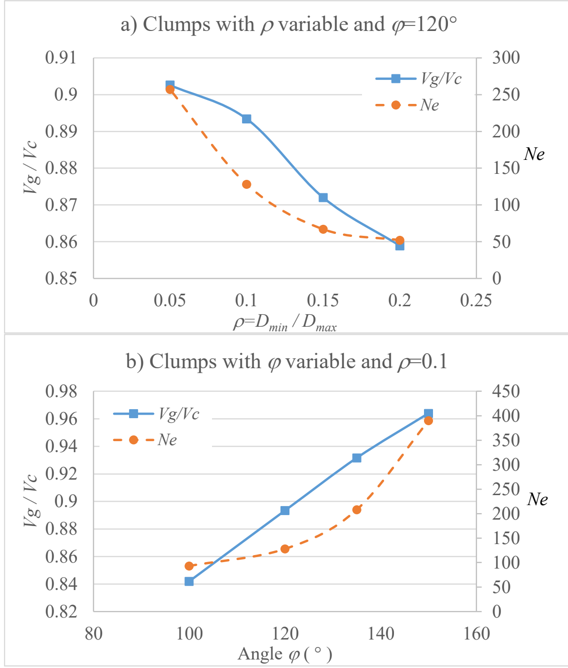

Figure 2. Approximation of a cube with clumps of spheres: a) effect of ratio ρ, b) effect of angle φ.

For this reason, in this research clumps whit the shape of tetrahedra, cubes, octahedra, dodecahedra, icosahedra, square plates and regular quadrangular prisms are used. Figure 3 show an example of each polyhedron represented by a clump of spheres, using the same parameters adopted in the representation of the cubes.

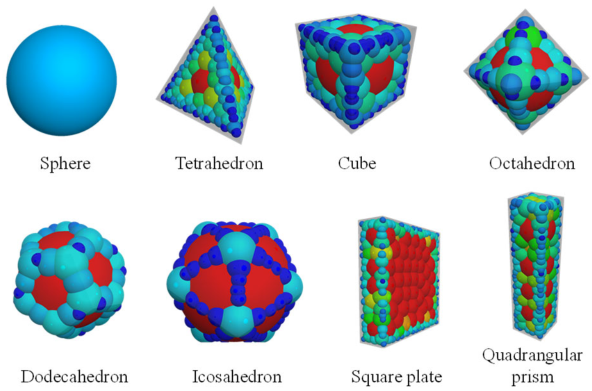

Figure 3. Shape of the particles used in this research

4.2 *Mechanical interaction among grains*

In numerical simulations of granular media by the Discrete Element Method (DEM), the interaction between particles occurs at the contact points according to a contact model. Granular materials of interest in geotechnics are typically frictional, so a linear contact model is adopted (Cundall and Strack, 1979).

To represent rigid grains and reduce the effect of the roughness induced by the clumps, stiffness coefficients $k_n = 10^7$ N/m, $k_s = 5.0^6$ N/m respectively. Friction coefficient $\mu = 0.7$ are considered in the simulations as representative for mineral grains (Cambou, 1974). It is important to note that, several studies (Zhang *et al*., 2001; Sánchez *et al*., 2015; Auvinet and Sánchez, 2023) have shown that higher values of porosity in granular media are obtained with higher values of friction coefficient.

4.3 *Creation of granular samples*

Currently, there are several methods for creating granular samples (Zhang *et al*., 2001; Isola, 2008), each with its own effects on the initial structure. The method chosen should be the one best suited to the objectives of the problem being studied. In this work, following procedure is implemented as representative of vertical placement by gravity as is done in many experimental works (Oda, 1972), and it is shown in Figure 4:

1. A container in the shape of a parallelepiped is created with a height much greater than that of the granular sample to be obtained.
2. Given a number of particles, their size is easily obtained by assuming an "*a priori*" porosity value of final assembly and dividing the volume of the sample solids by the number of particles in the simulation.
3. A set of particles are generated with random positions within the container space, without intersections between them and without intersections with the container.
4. These particles settle down by gravity. They interact with each other and with the container according to the contact model adopted until static equilibrium is reached.
5. Eventually steps 3 and 4 are repeated to create the granular sample in stages (García *et al*., 2009).

There are several criteria for accepting that a granular sample is in equilibrium. For example, in this work, this occurs when the sum of forces in the system is zero with an error of 10^{-5}.

The size of the simulated samples must be at least equal to the representative elemental volume (REV), that is, the minimum volume required for a property (porosity in this work) measured in it to be representative of the medium.

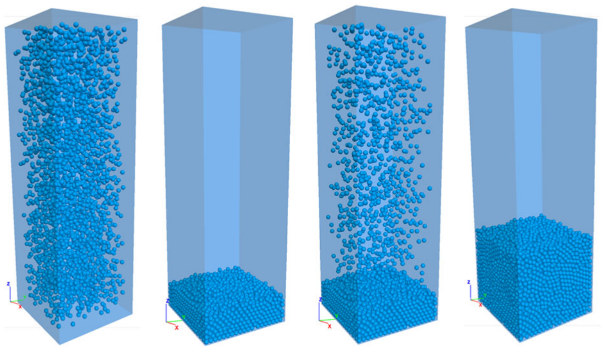

Figure 4. Simulation procedure for creating granular samples

Using the theory of random fields (Matheron, 1967), Auvinet (1986) and Auvinet and Bouvard (1988) studied the variance, $var[n_V]$, of the local porosity associated with a volume V in a granular sample. A characteristic function $K(\underline{X}) = 1$ is introduced if $\underline{X}$ belongs to the pores and $K(\underline{X}) = 0$ if $\underline{X}$ belongs to the solids. Thus, it is shown that the variance, σ_{nV}, decreases when volume V of the sample increases according to the Equation (2). This phenomenon is known as the "*geometric scale effect*" and can be used as reference to obtain the REV.

$$var[n_V] = \frac{1}{V^2}\int_V\int_V C_K(\underline{X},\underline{X}')\,dXd\underline{X}' = \sigma_{n_V}^2 \tag{2}$$

$C_K(\underline{X},\underline{X}')$ is the autocovariance of the characteristic function for points $\underline{X}$ and $\underline{X}'$.

For homogeneous materials with spherical particles, Auvinet (1986) presents the numerical solution to assess the geometric scale effect, $var[n_V]$, in a parallelepiped with edges a, b and c (Equation (3)).

$$var[n_V] = \frac{1}{(abc)^2}\int_0^a\int_0^b\int_0^c dx\,dy\,dz \int_0^a\int_0^b\int_0^c n(1-n)\,exp\left(\frac{-s_3 h}{4n(1-n)}\right)dx'dy'dz' \tag{3}$$

Being n: porosity of the medium, s_3: specific surface of the medium, and h: distance between two points $\underline{X}$ and $\underline{X}'$ with coordinates (x, y, z) and (x', y', z') within the medium.

It is intended that the simulated samples present a volume large enough for the σ_{nV} variance to be negligible, but small enough to be able to be analyzed numerically. *A priori* and due to computational limitations, samples with 5,000 identical polyhedra are proposed.

5 POROSITY OF SIMULATED GRANULAR SAMPLES

Once a granular sample is built, porosity is evaluated in a cubic space centered on the sample, called the central core. The position of the core makes it possible to avoid boundary effect (Auvinet, 1986; Aste *et al*., 2005), which consists of an increase in porosity in the vicinity of the container walls. The dimensions of the central core are half the width of the simulation container.

Table 1 shows the relevant characteristics of the simulated samples. The samples of plates and prisms are accompanied by a suffix indicating the height/width ratio of their polyhedra. Figure 6 and Figure 6 show some central cores.

Table 1. Characteristics of simulated granular samples.

Sample	*Vp/Ve*	*Ne*	*l/a*	*n*	*σ**
Spheres**	1.00	30,000	13.8	0.428	0.000495
Tetrahedra	0.123	550,530	4.61	0.543	0.000498
Cubes	0.368	630,912	9.41	0.475	0.000499
Octahedra	0.318	591,690	7.32	0.490	0.000500
Dodecahedra	0.665	429,044	18.5	0.461	0.000498
Icosahedra	0.605	674,782	12.2	0.448	0.000497
Plates 1/8	0.083	1,021,413	4.71	0.688	0.000463
Plates 1/4	0.161	845,839	5.93	0.578	0.000494
Plates 1/2	0.283	697,890	7.47	0.501	0.000500
Prisms 2	0.260	718,142	5.93	0.498	0.000500
Prisms 3	0.157	817,920	4.52	0.558	0.000497
Prisms 4	0.100	1,197,534	3.73	0.588	0.000494

Where: *Vp/Ve*: Volume of a polyhedron / Volume of its circumscribed sphere, *Ne*: Number of spheres in the sample, *l/a*: length of the central core / major edge of the polyhedron (for spheres a is the diameter), n: porosity of the granular sample, *Standard deviation calculated with expression 1, and **Standard deviation σ_{nV}=0.0095 calculated with expression 3.

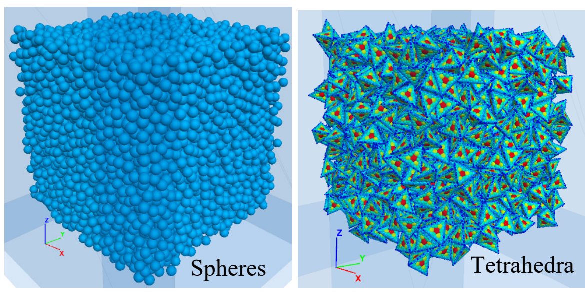

Figure 5. Central core of two simulated samples.

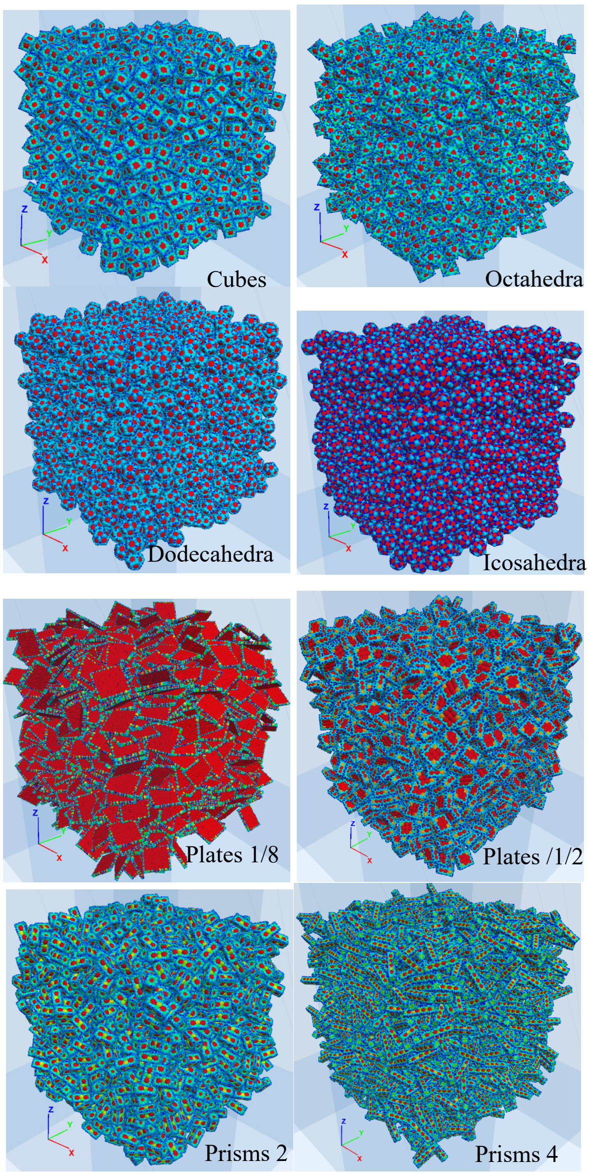

Figure 6. Examples of central core of several simulated samples.

In Figure 7 the variation of local porosity with the size of the central core volume in a granular material is shown. If the volume is small, of the same order of magnitude as the volume of the grains, values of local porosity are obtained that can differ significantly from the actual porosity of the medium. As the volume of analysis grows (l/a grows), the measured porosity tends to a constant value.

For samples of spherical grains in Figure 7 a), the confidence interval $n \pm \sigma_{nV}$ is included. It is accepted that the variation in porosity (σ_{nV} = 0.00095) from one sample to another is negligible for the size of the central core (l/a=13.8) adopted in these analyzes, so the porosity n=0.428 is representative of spherical particles materials.

In samples of polyhedra, it is difficult to isolate the geometric scale effect, and it is not possible to quantify the error associated with the sample size. By way of example, on the Figure 7 b), the porosity evaluated in three samples of cubes and in three samples of prisms is presented. In each type of material, the porosity tends to a constant value, with differences of less than 0.5% from one sample to another in the largest analysis volume.

Evaluated porosity in the different materials, as well as the variation interval ± 0.5%, is presented graphically in Figure 8.

It is observed that the sample of spheres presents the minimum porosity. This can be explained because the vertices of the polyhedra open the granular structure.

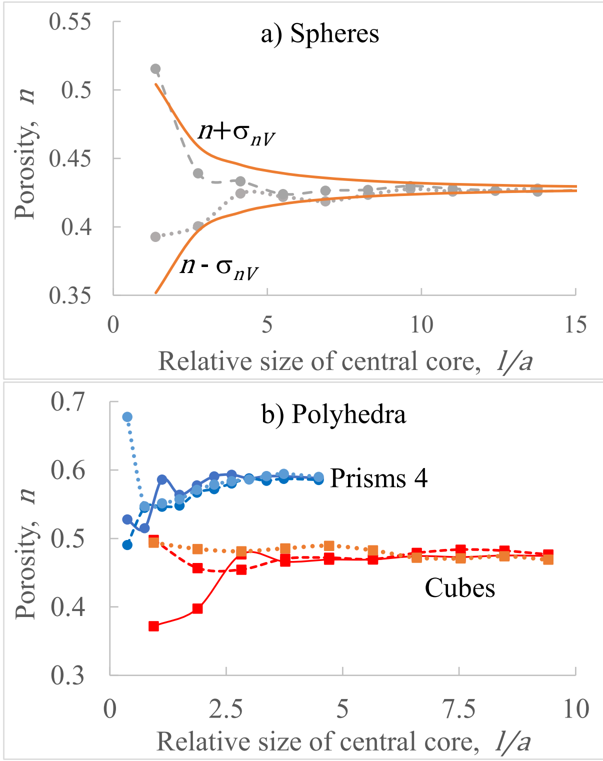

Figure 7. Typical variation of local porosity assessed in the central cores of different sizes

In the simulated samples of regular polyhedra, as is shown in Figure 8 a), the trend indicates that the porosity decreases when the volume of a polyhedron (Vp) fills a greater proportion of the volume of its circumscribed sphere (Vcs). Thus, the material of tetrahedra is more porous than that of cubes, octahedra, etc. In the literature (Teich *et al*., 2016), porosity has been associated to more complex geometric factors, but no better trends are obtained.

The porosity of samples of plates and prisms increases as the "height/width" ratio of these polyhedra moves away from unity (Figure 8 b). The porosity can be expected to approach unity when the height/width ratio tends to zero or infinity. In the other hand, the minimum porosity corresponds to the sample of cubes.

With respect to plates and prisms granular samples, it is also noted that porosity decreases when the polyhedron fills a larger fraction of its circumscribed sphere, but a much greater dispersion is obtained than for regular polyhedra.

The results obtained in this research show that the porosity of granular materials is strongly affected by the geometry of the grains. Although the results are not definitive, marked trends are obtained that can be considered as a reference to study granular materials composed of non-spherical particles. These trends must be useful in multiple practical problems and in particular, in Geotechnics, for example, for the design of light embankments for settlement control (Auvinet and Sánchez, 2020), breakwaters and others.

This experiment can be extended by considering different friction coefficients, different grain size distributions for particles of the same shape or by mixing polyhedra. Regular polyhedra can help study materials like sands, while plates can be used to study clays.

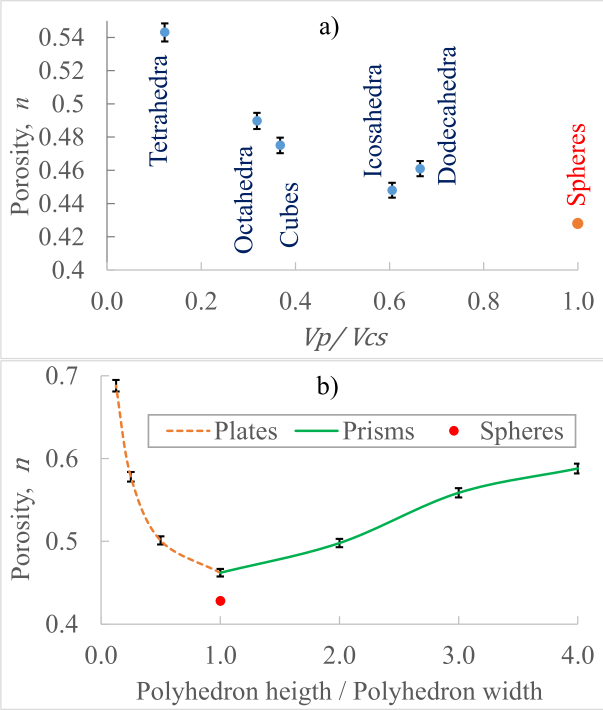

Figure 8. Porosity of random assemblies composed of identical polyhedra. a) Regular polyhedra and b) Plates and prisms

6 CONCLUSIONS

In this work, the inherent porosity of granular media constituted of identical grains with shape of polyhedra is analyzed. Spheres, tetrahedra, cubes, octahedra, dodecahedra, icosahedra, square plates, and regular square prisms are considered as elementary study.

Granular samples are constructed randomly using the discrete element method and a specialized algorithm to create clumps of any shape. It is accepted that the clumps interact at their contact points according to an elastic linear model with friction.

The porosity of the simulated materials is assessed with the Monte Carlo technique, guaranteeing that the error associated with the estimation method does not affect the third decimal point of the porosity. The same technique is used to evaluate the quality in the representation of polyhedra, for example, it is observed that it is possible to represent at least 90% of the volume of a cube.

Regarding the granular material of cubes, with a representation of 96% of the volume of each cube, a porosity of 1% greater than in the previous case is obtained. This is explained by the fact that the more pointed edges of the cubes open the pores. However, the computational work involved in this small improvement is excessive.

The error in the estimation of local porosity associated with the size of the granular samples studied (scale effect) can only be evaluated for spherical particles, where it is detected that the third decimal number is valid, σ_{nV} = 0.00095. By repeating some samples of polyhedra, differences of 0.5% were obtained in porosity from one sample to another.

Therefore, it is concluded that the study of the porosity of granular media involves various sources of error, so it is very important to proceed meticulously before exploring irregular grain geometries.

The simulations effected in this work show that the geometry of the grains considerably affects the porosity of a granular material. The porosity of the material constituted of spheres is the minimum of all the cases analyzed. The tetrahedron material exhibits the highest porosity among samples composed of regular polyhedra. For square plates and regular square prisms, granular media are more porous when the height differs more from the other two dimensions (length and width).

It is concluded that the porosity of the samples studied is higher when the polyhedron fills a smaller proportion of the volume of its circumscribed sphere.

Trends found in the porosity of granular media formed by polyhedra can be relevant in multiple areas of basic science, industry, and engineering. This work should be rigorously improved and extended to study the porosity of irregular particle materials such as soils.

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