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Specific volume of the most probable disordered sphere packings

Calixtro Yanqui [1,*]

[1]Civil Engineering Department, National University of Saint Agustine of Arequipa, Peru

Abstract. Most granular materials are made of randomly distributed grains. Theoretical and experimental studies, carried on by several authors, have shown that minimum and maximum specific densities of random packings vary primarily according to the type of strain, such as vertical compression and horizontal shear. In this regard, there are two approaches; the statistical geometry of packings, and the statistical mechanics. The fundamental objective of these theories is to settle down the limiting values, called RLP and RCP. […]However, in the mechanics of granular materials, intermediate values are also important. For this reason, in this paper, a model for packings is proposed, based on elementary probability. The angles of a parallelepiped formed by eight spheres of equal size are taken as random variables, and the probability density function is assumed to be uniform. Specific volume of three-dimensional packings subject to two or three dimensional strain are calculated using conditional and joint probabilities, respectively.

1 Introduction

Soils technological properties, such as liquefaction potential, compaction, shear and compression strains, among others, are better understood using sphere packings. The simplest model that fulfills this purpose is the regular packing of spheres, in which the angles of the primitive cell can be related to the applied stress and strain. A more realistic model takes into account the random distribution of the grains in the sample [1]. According to Bernal [2], the description of this model can be achieved by following two paths: the statistical geometry of the packings and the statistical mechanics. The first path is based on the average number of spheres in contact with any given sphere, as function of the radial distance. [3][4]. In this case, the experimental data fit well with the Gauss distribution. Also, scalar variables are considered to characterize disordered packings, such as the volume fraction and the order metric, which includes various translational and orientational parameters, [5]. The second path treats granular materials using the formalism of the statistical mechanics by substituting the temperature by a parameter called compactivity, and the energy, by an equiprobable volume ensemble, which is a close system that takes up all mechanically stable configurations [6][7]. Some authors suggest that better results are obtained by combining both methods [8][9]. A different statistical geometric approach is proposed in this work, applying the elementary theory of probability to the angles of the Bravais triclinic lattice, generalizing the simple averaging method presented in previous works [10][11].

2 Regular packings

A triclinic lattice comprises most of the Bravais arrangement of homologous points, as particular cases. The primitive cell of this lattice is a parallelepiped, each vertex of which is the center of a hard sphere, in contact with some spheres of the other vertices (Fig. 1a). By convenience, the parallelepiped is defined by three edges, of lengths a, b, and c, and two angles, α and ζ, which represent the crystalline or polar angle of the horizontal rhombic base, and the azimuthal angle of the sphere pair with the gravity direction, respectively (Fig. 1b). The isostatic mechanical equilibrium of each sphere is ensured by the three reaction forces that coincide with three of the contact lines between the frictionless spheres.

In numbers, the total volume of the prismatic element is $V=abc \sin\alpha \cos\zeta$. Because of the symmetry of the packing of spheres, angle α varies between two physical limiting values, 60° and 90°, corresponding to

* Corresponding author: cyanqui@unsa.edu.pe

a hexagonal and square bases, respectively. In addition, the sum of the eight spherical trihedrons, defined by the three concurrent edges, and contained in the parallelepiped, is equal to the volume of a sphere of diameter D: $V_s = \pi D^3/6$.

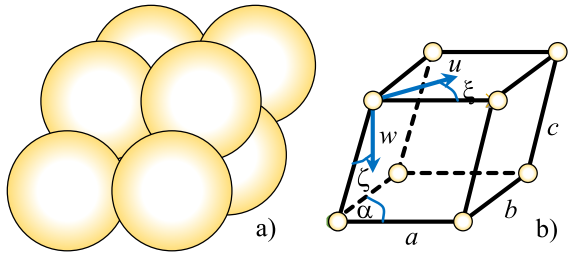

Fig. 1. Basic element of a hard sphere packing: a) volumetric representation, b) parallelepiped drawn by the centers of the eight spheres.

The two extensive quantities may be related in different ways; for example, by the specific density, also named volume fraction, $\phi=V_s/V$, or by the specific volume, $\upsilon=V/V_s$. The latter relationship is used in this approach:

$$\upsilon = \frac{6abc}{\pi D^3}\sin\alpha\cos\zeta \quad (1)$$

because it maintains linearity with the trigonometric functions of the crystalline angles, and its integration yields close form functions. In this formula, the lengths a and b are not constant, but depend on the packing angles, regarding the type of strain. According to the type of experimental method, two kinds of elementary strain can occur: horizontal shearing and vertical compression, defined by the vectors $\boldsymbol{u}$ and $\boldsymbol{w}$, respectively, but the specific volume, υ, does not depend on the direction of the displacement, ξ.

2.1 Packing strained by horizontal shear

In this case, all edges are lines of contact, and the packing deformation occurs by displacement of the upper layer with respect to the lower layer, following the direction of the vector $\boldsymbol{u}$. Due to a horizontal shear force, spheres move respect each other, preserving the prismatic shape of the cell, and varying the angle of distortion β, which coincides with the azimuthal angle ζ. That is why $\zeta = \beta$. The shear strain is called two-dimensional (2D), if the edges b and c are perpendicular to each other, and the movement of the upper sphere follows the direction $\xi=0$ (Fig.2.a). When the displacement of the upper layer occurs along the horizontal diagonal of the layer, the shear strain is considered three-dimensional (3D), and the displacement direction is $\xi=\alpha/2$. In both of the cases, isostatic equilibrium requires that $a=b=c=D$. Then:

$$\upsilon = \frac{6}{\pi}\sin\alpha\cos\beta \quad (2)$$

Table 1. Volume fraction of limiting shear regular packings.

	β_{min}°	α=60°	α=90°	β_{max}°	α=60°	α=90°
2D	0	0.605	0.524	30	0.698	0.605
3D	0	0.605	0.524	35.26	0.740	--
3D	0	0.605	0.524	45	--	0.740

The mathematical root $\beta=0$ yields packings made of columns, and two minimal limiting volume fractions; both of them related to an unstable isostatic condition. Close packings are achieved by the physical limits of the angles. For the 2D strain, they are associated to two different values, one of which is 0.698, coinciding with the dodecahedral volume fraction of the Voronoi tessellation [9]. For both of the 3D strained packings, the maximum volume fraction is 0.74 (Table 1).

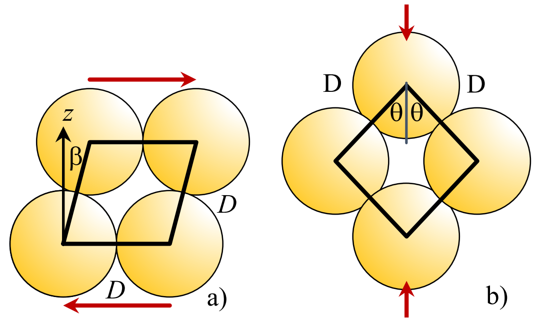

Fig. 2. Lateral view of 3D packings submitted to 2D strains: a) shear, and b) compression.

2.2 Packing strained by vertical compression

For the two-dimensional strain (2D), any sphere of the upper layer is in contact with two spheres of the lower layer and is strained by vertical indentation, following the displacement vector $\boldsymbol{w}$ (Fig.2.b). The inclination with respect to the vertical is defined by the angle of obliquity θ, that coincides with the azimuthal angle ζ, so that $\zeta = \theta$. In this case: $a=2D\sin\theta$, $b=c=D$. Then

$$\upsilon = \frac{6}{\pi}\sin\alpha\sin 2\theta \quad (3)$$

Comparison of equations (2) and (3) for 2D strain yields the relation $\theta=\pi/4-\beta/2$, which sometimes has been confused with the Mohr-Coulomb failure angle. In three-dimensional (3D) compression, contact lines draw an asymmetric tetrahedron, made of an edge and two face diagonals, except for the octahedral packing. Now, the angle θ has another mechanical meaning, but the relationship $\zeta=\theta$ still remains. The edge lengths are given by: $a=b=2D\sin\theta\cos(\alpha/2)$, and $c=D$. Then

$$\upsilon = \frac{48}{\pi}\sin\frac{\alpha}{2}\cos^3\frac{\alpha}{2}\sin^2\theta\cos\theta \quad (4)$$

Table 2. Volume fraction of limiting compression regular packings

	θ_{max}°	α=60°	α=90°	θ_{min}°	α=60°	α=90°
2D	45	0.605	0.524	30	0.698	0.605
3D	54.74	0.524	0.680	35.26	0.74	--
3D	54.74	0.524	0.680	45	--	0.74

3 The most probable packing

In most of the problems, a sample, Ω, contains a very large number of spheres randomly located in a container, depending primarily on the aggregation process and the boundary conditions. The sample is assumed to be a set of packings whose inherent angles varies randomly within their physical domain, independently of their location and orientation. The

Gauss definition of the most probable value, weighted by a uniform probability density function, is used to find the expected specific volume [12].

Considering α and ζ as random variables, the bivariate histogram ordinates can be described by a joint probability density function: $f=f(\alpha,\zeta)$, defined in the domain of physically possible regular packings: $\pi/3 \le \alpha \le \pi/2$, and $\zeta_1 \le \zeta \le \zeta_2$. Particularly, in the absence of further information, all packings contained in the assemblage can be considered equally probable. This implies that the probability density function $f(\alpha, \zeta)$ is uniform, and can be described as the product of two random functions: $f(\alpha,\zeta)= f_1(\alpha)f_2(\zeta)$. If the angle ζ is known in advance, the specific volume of a random packing defined by angle α is said to be conditional and is denoted by $f(\alpha|\zeta)$. The same is true when α is given in advance, in which case, the probability function is denoted by $f(\zeta|\alpha)$.

In addition, specific volumes described by equations (2), (3) and (4) are also the product of two independent trigonometric functions $h_1(\alpha)$ and $h_2(\zeta)$, and may be symbolized as: $\upsilon=\upsilon(\alpha,\zeta) =(6/\pi)h_1(\alpha)h_2(\zeta)$. This property, together with the uniform probability density functions, allows for finding the mathematical expectation of the most probable specific volumes. The discussion and the good correlation of these results with the experimental data are presented in a parallel paper [13].

4 Azimuthal random packing

In this type of probable packing, the angle α is a previously determined random variable, and angle ζ is the random variable that allows for calculating the average of the trigonometric function h_2. This statement corresponds to the conditional probability of ζ given α: $f(\zeta|\alpha) = f(\alpha,\zeta)/f_1(\alpha) = f_2(\zeta) = 1/(\zeta_2-\zeta_1)$.Therefore, the expected value of the specific volume of the random packing is the definite integral of the azimuthal conditional probability:

$$E[\upsilon(\zeta)] = \frac{6}{\pi}\frac{h_1(\alpha)}{\zeta_2-\zeta_1}\int_{\zeta_1}^{\zeta_2} h_2(\zeta)d\zeta \qquad (5)$$

In this equation, the limits of integration are defined by the symmetry of the corresponding regular packing, regarding the type of strain. Indeed, in this range of values of ζ, the probability distribution function of the measured azimuthal angles is maximum, almost constant, and weak dependent on friction [4].

Table 3 presents the expected values of the specific density as a function of the angle polar α. It also shows the particular expectations for the limiting values: α=90° and α=60°, associated to loose and close packings, respectively. The calculated values are comparable to those fractions obtained theoreticaly by Song et al. [8]. They showed that the specific volume ensemble is inversely proportional to the number of contacts of the sphere. Then, establishing that geometrical and mechanical coordination numbers correspond to each other, they found a density fractions of 0.536 and 0.634, for coordination numbers of 4 and 6, associated to infinitely rough and zero friction spheres, respectively. Aste et al. [3], found 0.555 and 0.645, assuming a radial distribution and a limiting distance of 1.255 diameters of the equal-sized spheres. These values are similar to those of packings subject to 3D-shear.

Table 3. Specific volume and limiting volume fractions of azimuthal random packings.

Strain	Expected specific volume $E[\upsilon(\zeta)]$	α=90°	α=60°
2D-shear or compression	$\frac{18}{\pi^2}\sin\alpha$	0.548	0.633
3D-shear	$\frac{2\sqrt{3}}{\pi\sin^{-1}(1/\sqrt{3})}\sin\alpha$	0.558	0.644
3D-compression	$5.7154\cos^3\frac{\alpha}{2}\sin\frac{\alpha}{2}$	0.539	0.700

5 Polar random packings

When the random variable ζ is already given, the probability function becomes univariate and depends only on α. This condition corresponds to the conditional probability of α given ζ: $f(\alpha|\zeta) = f(\alpha,\zeta)/f_2(\zeta)=f_1(\alpha)=6/\pi$. The expected value of the specific volume can be calculated from the expression:

$$E[\upsilon(\alpha)] = \frac{36}{\pi^2}h_2(\zeta)\int_{\pi/6}^{\pi/2} h_1(\alpha)d\alpha \qquad (6)$$

In this case, the integral limits are the same, regardless of the packing type, but the limiting packings are given by the azimuthal random packing angle, regarding that subscripts 1 and 2 correspond to the loose and close states, respectively.

Table 4. Specific volume and limiting volume fractions of polar random packings

Strain	Espected specific volume $[\upsilon(\alpha)]$	Loose packing	Close packing
2D-shear or compression	$\frac{18}{\pi^2}\cos\beta$	0.548	0.633
3D-shear	$\frac{18}{\pi^2}\cos\beta$	0.548	0.672
3D-compression	$\frac{45}{\pi^2}\sin^2\theta\cos\theta$	0.570	0.620

The most probable specific volumes are described by the equations given in Table 4, in which the values corresponding to the loose and close packings are also presented. It is worth to note that, for compression, these specific densities coincide with those of the statistical mechanics, that yields the following specific densities [14]: 0.58, for the initial condition, 0.62, for an infinite compactivity, and 0.64, for a null compactivity.

Of all the possible diagrams, the one that relates the volume fraction to the polar angle for 3D shear strain, is given in Fig. 3; in which, the important issues are the curve of the most probable volume fraction limited by 0.548 and 0.672, and the curve of the close regular packings whose maximum and minimum volume fractions are 0.74 and 0.698, respectively.

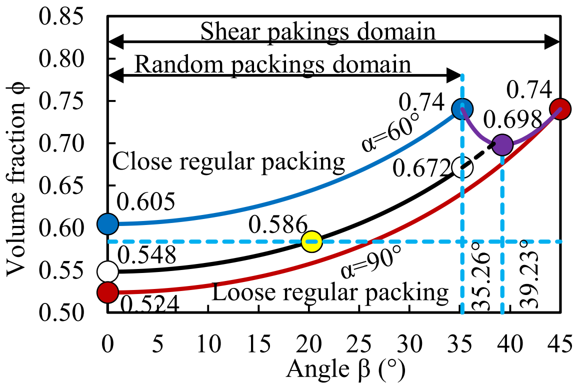

Fig. 3. Volume fraction versus azimuthal angle for a 3D shear strain. Physical and mathematical most probable packings are represented by continuous and discontinuous black line, respectively. Limiting values are symbolized by dots, together with the joint random value (yellow).

6 Joint random packings

The expected specific volume of the completely disordered packing is described by the uniform joint probability density function, which depends on the random variables α and ζ:

$$E[\upsilon(\alpha,\zeta)] = \frac{6}{\pi}\int_{\alpha_1}^{\alpha_2}\cdot\int_{\zeta_1}^{\zeta_2} h_1(\alpha)h_2(\zeta)f(\alpha,\zeta)d\alpha d\zeta \qquad (7)$$

The expected specific volumes are 0.574 and 0.586 (Fig. 3) for 2D and 3D strains. These values have been obtained experimentally by pouring the spheres to the air into a container. They have been validated by means of the Monte Carlo simulation [15]. This suggests that around ϕ=0.58 an important phase change occurs [4], separating the loose and close branches of the most probable value. Consequently, if only the branch of close packings is considered, the joint random volumen fraction is 0.64, for the RCP. It is also worth to mention that Brouwers [16] found good results for hard discs packings in a plane by means of the joint probability of the volume fraction.

7 Conclusions

The comprehensive view of the most probable packing model leads to the conclusion that a random variable can be interpreted as a degree of freedom, and the given variable in conditional probability is a restriction. Accordingly, the joint probability describes the free pouring of spheres, while the conditional probability also includes, for example, vertical vibration. For this reason, 0.58 is the volume fraction corresponding to the totally disordered packing [9], associated to the critical state in soil mechanics and the phase transition in glasses. Any other looser or closer packing implies some degree of order until crystallization, and the azimuthal and polar limiting angles represent phase changes. For example, the volume fractions for compression strain packings are 0.548, 0.62, 0.64, 0.67 and 0.70, related to known experimental restrictions, such as: enforce by reducing the velocity of the spheres fall, tapping, vertical vibration, batch-wise feeding, and partial feeding, respectively. These values, although are protocol-dependent, do not come from the Torquato et al. model [17], which is based on the minimization of an order parameter, opposite to the randomness.

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