Aggregate Packing And Coordination Number – A Statistical Approach

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Synopsis

Most of the past studies of aggregates as used in pavement engineering have focused on large-scale observations of the material's properties, trying to estimate and predict them as a whole using models that, often, descend from purely theoretical considerations. Therefore, the increased ability to describe overall performance sometimes does not explain the underlying causes. As a material's macroscopic behaviour is in some way the outworking of particles interaction, it is unquestionable that a deeper understanding of these interactions and their effects is desirable.
For this reason, the authors' attention has focused on aggregates from a "geometric" point of view, aiming to link the general mechanical properties with small-scale characteristics. In this paper, the possibility of estimating the coordination number (number of contact points that an aggregate particle has with other aggregate particles) within the aggregate (either as an average or as a distribution) is considered of high importance, as other researchers have shown that it has a major influence on aggregate durability and permanent deformation. At this early stage, the study must be conducted in a theoretical way considering an "easy" material whose particles are all spheres. Once a conclusion is achieved with this simplification, the research will go further considering the real particles' shape using parameters such as sphericity, angularity and roundness.
As part of this more general packing theory, the most important step is to predict the coordination number for a random distribution of equal spheres, which is the main subject of this paper. If this target is accomplished, moving this knowledge to the multi-size case will just be one step forward.
It must be said that this study has always been conducted from an engineering point of view rather than from a mathematical one. The authors' ultimate aim is to produce a useful tool, not a theorem.
Coordination number is recognized to be a function of the aggregate's geometry: particle shape, grading and compaction degree are the factors that determine the spatial configuration of this system. If the considered material consists of spherical particles of the same size, two of these three factors disappear and coordination number becomes a function only of the compaction degree. Two different approaches were taken to identify this relationship: random generation of spheres on the surface of a central one and random box filling with equal spheres. Both these methods aim to generate a large data set from which to derive statistical observations on packing variability.
The results obtained from the two methods enable the authors to clearly define the role that packing degree (in the form of solid ratio) has in affecting the sphere assemblies' arrangements. The first method provided a statistical description of the contact points' distribution on particle surface, while the second method delivered equations for predicting coordination number within an assembly of given solid ratio.

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INTRODUCTION

As a result of particle interaction within an unbound granular pavement material (UGM) when subjected to an external loading, one is able to observe its deformational behaviour and the changes in its mechanical properties. A UGM's deformation is generally divided into permanent and resilient elements: the first one is broadly known to be due to rearrangement and fracture of the particles under each loading cycle, the second reflects the real elasticity of the grains and is recovered with unloading. Each complete cycle of loading and unloading draws a hysteresis loop in the stress-strain plane, which represents the loss of energy in terms of work carried out on the volume element: a great part of this energy is transformed into heat, some is used to damage the particles and only a small part is exploited to cause displacement.

Thom and Brown [1] investigated the influence of grading and dry density on aggregate behaviour, performing repeated loading triaxial tests on specimens of various gradings and 3 different degrees of compaction. They observed a substantially constant resilient strain with respect to these parameters, with a slightly increasing trend as the aggregate became more compacted. This seems to indicate that the material itself basically rules the resilient properties, without any major influence from the volumetric distribution. Of higher relevance were their results about permanent deformation: "resistance to plastic strain is similar for all gradings when heavily compacted but, if the material is less well compacted, uniform grading has better resistance". Shear strength is also greatly improved by increasing the degree of compaction. Permanent deformation and shear strength can then be considered to be highly influenced by geometric factors such as grading, void ratio, degree of interlocking and friction angle between the particles.

A change in grading and void ratio can be expected to result in a different value of the coordination number (number of contact points between a particle and its neighbours) leading to a different stress distribution over the particle's surface: a coarse aggregate consisting of grains of the same size with a small fine fraction will load each particle with higher tensile stresses than if the same particles were conveniently surrounded by an appropriate number of smaller particles. As shown by McDowell [2], "the probability of fracture is a function of applied stress, particle size and coordination number. When the effect of coordination number dominates over particle size in determining the probability of fracture for a particle, the resulting particle size distributions are fractal in nature. By choosing appropriate particle parameters, it is possible to obtain normal compression curves which resemble those found experimentally". ([3] and [4])

Developing a tool to estimate the coordination number means, therefore, acquiring a deeper knowledge of the phenomena that rule the micro-mechanics of particles. This paper aims to clarify the relationship between coordination number and solid ratio (the proportion of a volume occupied by particles), separating it from the effects that particle shape and grading have on the aggregate spatial configuration. To do this, the geometrical properties of a material consisting of single-sized spherical particles have been studied from a statistical point of view.

The problem of spheres' packing involves many different branches of physics and mathematics, starting from the best way to stack oranges and including the coding and decrypting science. Most of the efforts have been concentrated on the study of single-sized spheres. Thus a variety of evaluations can be found in the literature that try to relate the mean coordination number to porosity ([5] and [6]), particularly for some "standard" packings. There are also some exact packing solutions for particular particle arrangements.

For multi-sized systems the determination of coordination number is much more difficult than for a system of equal spheres: the number of variables rapidly increases and so does the information required. For example, a binary mixture gives three types of contacts: large-large, large-small (small-large) and small-small, with each type of contact having its own distribution. Very little useful information can be found in the literature about these problems ([6] and [7]).

METHODOLOGY

Due to the three-dimensional nature of the problem, a statistical approach seems to be more suitable than a deterministic one. It is, in fact, impossible to uniquely relate a certain value of solid ratio with a single coordination number: different configurations of spheres (i.e. different coordination numbers) can easily end up with the same solid ratio. The only thing that is reasonable to look for is the statistic probability for a certain coordination number to appear for a given solid ratio. This is, therefore, the aim of this project.

Two different methods have been applied in order to reach a general overview. Both of them generate spheres' three-dimensional configurations giving, as an output, the coordinates of the spheres' centres in a Cartesian system, OXYZ, and the coordination number for each sphere. The solid ratio can then be calculated for each sphere as the ratio between the sphere's volume and the volume of its "Voronoi" cell.

In a system of spheres (*A*), the Voronoi cell belonging to one particular sphere (*a*) is defined as the total of the space's points which are closer to the centre of *a* than to the centre of any other sphere of the system *A*. To state it in another way, it is the smallest volume totally enclosed by the planes which are perpendicular bisectors of lines joining the centre of sphere *a* to all other sphere centres. This concept is illustrated by a two-dimensional example in Figure 1.

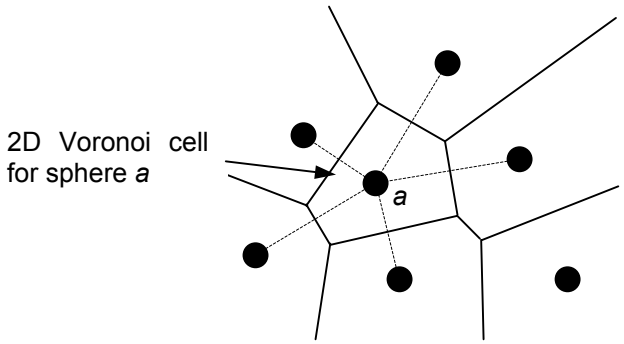

Figure 1: Voronoi construction in 2 dimensions

The modern use of the Voronoi construction began with crystallography, but since then it has become much more general proving its efficacy in disciplines like geography, ecology, and politics. Basically, it can be applied everywhere spatial patterns are analyzed to identify regions of activity or influence [8]. In the case of this study, it represents an excellent way to evaluate the portion of space "attached" to each sphere (Figure 2).

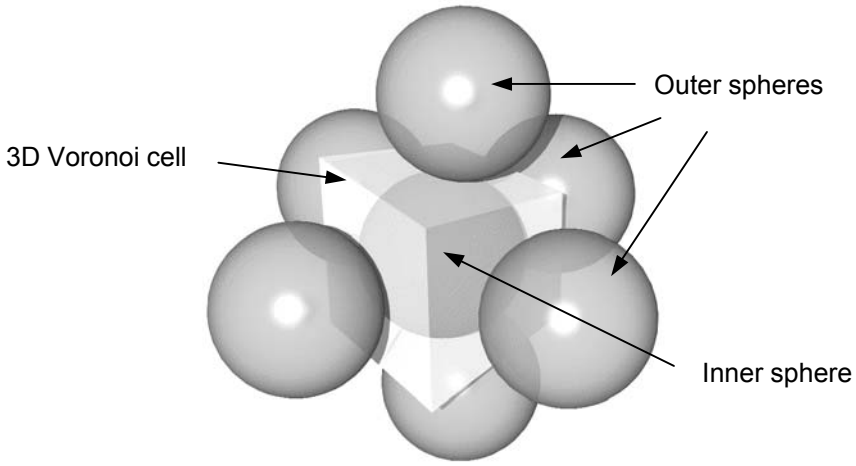

Figure 2: 3D Voronoi cell in a spheres assembly

Method 1: spheres on the surface of an inner one

The first method used has been an attempt to generate all the possible configurations of spheres around an inner one of the same radius. Each outer sphere is identified by its contact (or "kissing") point with the inner one, expressed in a spherical coordinates system centred on the inner sphere by the angles θ (longitude) and φ (latitude). To randomly generate the position of an outer sphere means, then, to produce a couple (θ; φ) indicating a kissing point on the surface of the central sphere. It is possible to demonstrate [10] that a statistically uniform distribution for those points can be achieved with θ and φ being taken as follows:

$$\theta = 2\pi u \qquad (1)$$
$$\cos\varphi = 2v - 1$$

with u and v being random real numbers between 0 and 1. It would be incorrect to select directly the spherical coordinates from the uniform distributions $\theta \in [0, 2\pi)$ and $\varphi \in [0, \pi]$ because the points would be weighted towards the "poles" of the inner sphere.

In order for the configuration to be geometrically acceptable, the chosen kissing point for the second (and subsequent) outer sphere must not permit the new outer sphere to overlap a previous outer sphere. The easiest way to check this condition is to impose that the distance between each pair of kissing points must not be less than one radius length (see Figure 3).

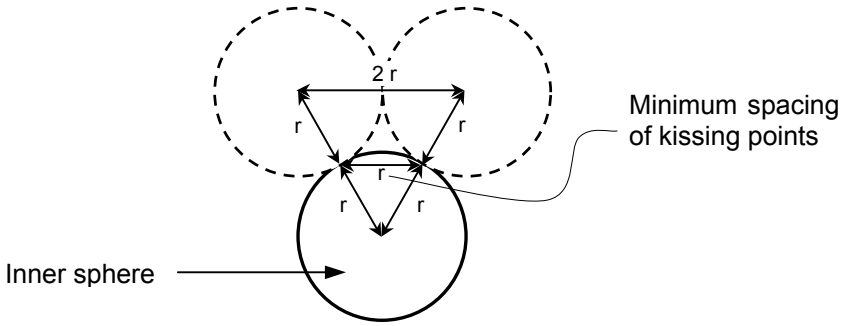

Figure 3: Non-overlapping condition

There are, basically, two different algorithms to deal with this aspect, which are as follows.

1st Algorithm
Intuitively, the most direct way is to:

- Pick one point;
- Calculate its distance from all the previously saved points: is it too close to any?
- YES, not acceptable, delete it;
- NO, acceptable, save it.

This simple algorithm has got two weak points that make it unsuitable for this study. First: it doesn't know when to stop. The maximum possible number of spheres that may be placed is 12 (an observation known as the "Kepler conjecture" since it was first observed by Kepler [8]). However, this number belongs to a situation when all the spheres are very well packed all together. Therefore, it is possible (and, as will be shown later, it is very likely to happen) that after having placed 8-9 spheres randomly there is actually no physical way to place the 10th one, and this is perfectly acceptable. This first algorithm is not able to check this condition, thus it would go on forever trying to reach 12. Second: as the number of saved points increases, the number of attempts and the time to find the next acceptable coordination point increases greatly. This way, in a trial made by the authors, it was found that a normal computer would take a day for 8 points and a month for 9! Considering that the main target is to produce many thousands of configurations, this work would have taken a few centuries!

2nd Algorithm
Instead of going on picking the points in the whole surface of the inner sphere, it is much better to randomly pick each n^{th} contact point only in the surface which remains available after having placed the previous n-1 points:

- Pick one point in the available area;
- Save it;
- Calculate the new available area.

In this way both the problems of the previous algorithm are solved. First: the program will run as long as there is still any available area on the sphere's surface, no matter what the number of placed spheres is. Of course, the maximum possible number is still 12, but we don't need to define this. Second: the algorithm doesn't need to make many attempts to pick a point, because it is just choosing it among the acceptable ones. Thus, with this new algorithm the required time to produce a full configuration is always few seconds.

Each placed sphere thus reduces the available area for subsequent coordination points as shown in Figure 4 for the plane case. Each new sphere placed will subtract (in the 2-D example) an angle equal to $1/3^{rd}$ of the total (i.e. 2π/3 radians) from the available places where subsequent kissing may occur. The new angle subtracted is allowed to overlap as much as $1/6^{th}$ of the total (i.e. π/3 radians) with the angle subtracted by previous placed spheres (see Figure 4d).

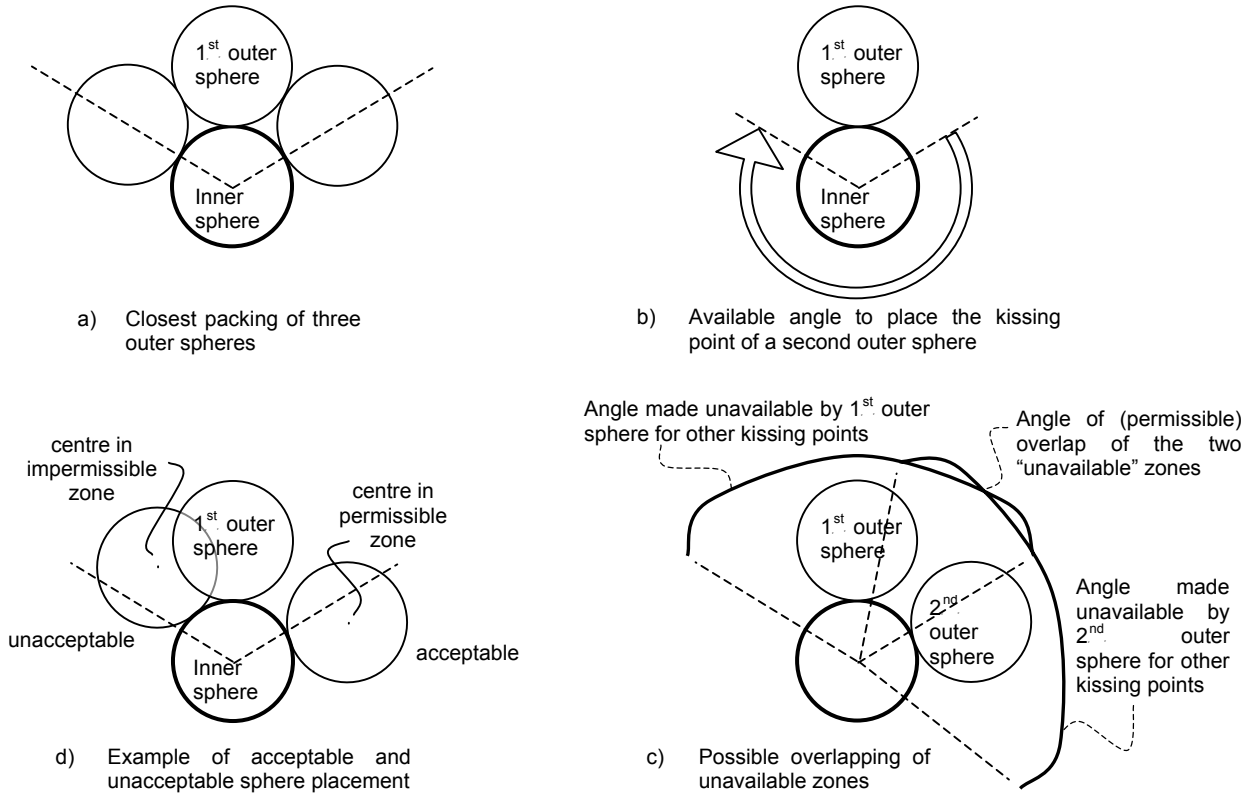

Figure 4: Concept of available angle and overlapping zone in 2 dimensions

Due to the transformation (1) introduced before, a relationship is established which uniquely links each polar pair (θ; φ) to the correct value of the transformed pair (u; v). The sphere's surface can then be exactly represented in a u-v space as a square of unit side as shown in Figure 5, where the shaded area is unavailable for the kissing point of the 4th outer sphere.

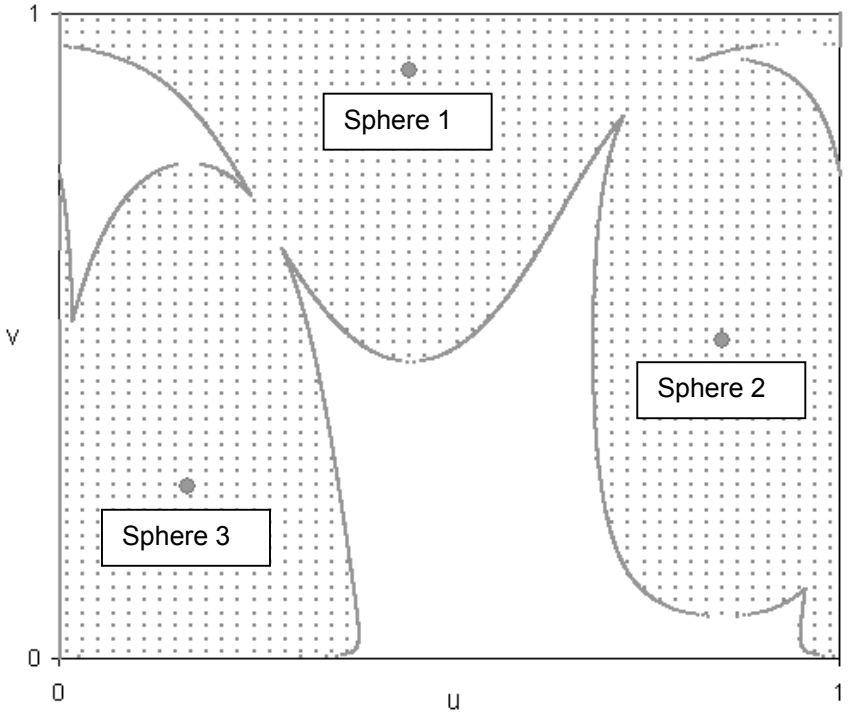

Figure 5: Representation of the inner sphere's surface in the u-v space

Moving from 2-D to 3-D the concept of available area does not change much: the angle becomes a cone around each ball and subtracts an area equal to 1/4$^{th.}$ but, of course, still allows overlapping (see sphere 2 and sphere 3 in Figure 5). Having already taken into account all the necessary restrictions, every single white zone that remains, even the smallest one, is suitable for a further kissing point.

Method 2: equal spheres in a box

The second method simulates the gradual filling of a cubic box with spheres of equal size, placing one at the time the new spheres in the depressions ("pockets") formed by the previous ones. The algorithm does not allow for any rearrangement of the spheres that takes place in the physical experiments due to sphere's weight. This does not represent a limit for the present study: as long as the authors aim to produce a random spheres' assembly, there is no need for this assembly to be subjected to any physical law. Particles rearranging themselves due to gravitationally induced movements or compaction, provided they still deliver a random packing, only increment the average solid ratio. Therefore, configurations with high solid ratios become of more relevance than those with lower ones.

As the target of this study is to analyse the whole range of possible solid ratios, and to associate coordination number with solid ratio, it is desirable to be able to fill the imaginary box in different ways to obtain different packings. Maintaining the random nature of this method, this can be done by the following deposition algorithm:

- Randomly drop a sphere inside the box;
- Place it in the lowest point ("pocket") available within a given distance (*d*) from the falling point.

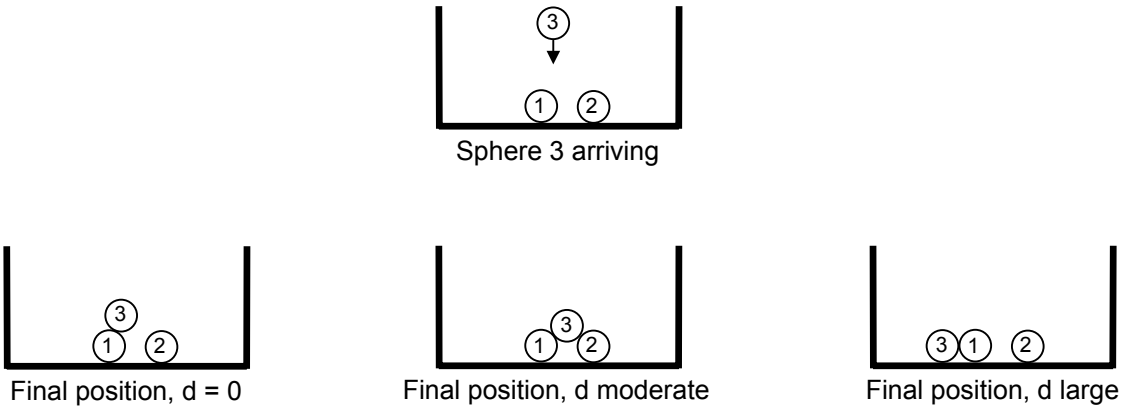

Figure 6: Different packings obtained varying parameter *d*

This way, it is easy to see (Figure 6) that the best packed configurations will be those produced with the largest *d*, because each sphere has been placed in the lowest possible point and, therefore, it is possible to fill the box with a larger number of spheres (Num), while when $d \rightarrow 0$ the spheres just "stick" where they fall, resulting in a looser packing. The obtained packings are, therefore, a function of *d* alone, while box size and sphere radius do not influence them. This concept is clearly shown in Figure 7 for the 6 different pairs of box size (b) and sphere radius (r) summarised in Tab 1.

Tab 1: Different side-radius pairs used to produce Figure 7

Analysis	Box's side (b)	Spheres' radius (r)	b/r	Av. Nroll
A	100	10	10	107
B	100	5	20	941
C	100	3	33	4417
D	50	5	10	105
E	30	3	10	101
F	60	3	20	915

Column "Av. Nroll" of Tab 1 refers to the average number (Nroll) of spheres that can be placed with a different algorithm that, instead of moving the dropped sphere to the lowest point within the range d, drops each sphere in the box and makes it roll down until a position of stable equilibrium is reached. As shown in Tab 1, this number is a function only of the ratio b/r, therefore it is suitable to normalise the data as presented in Figure 7.

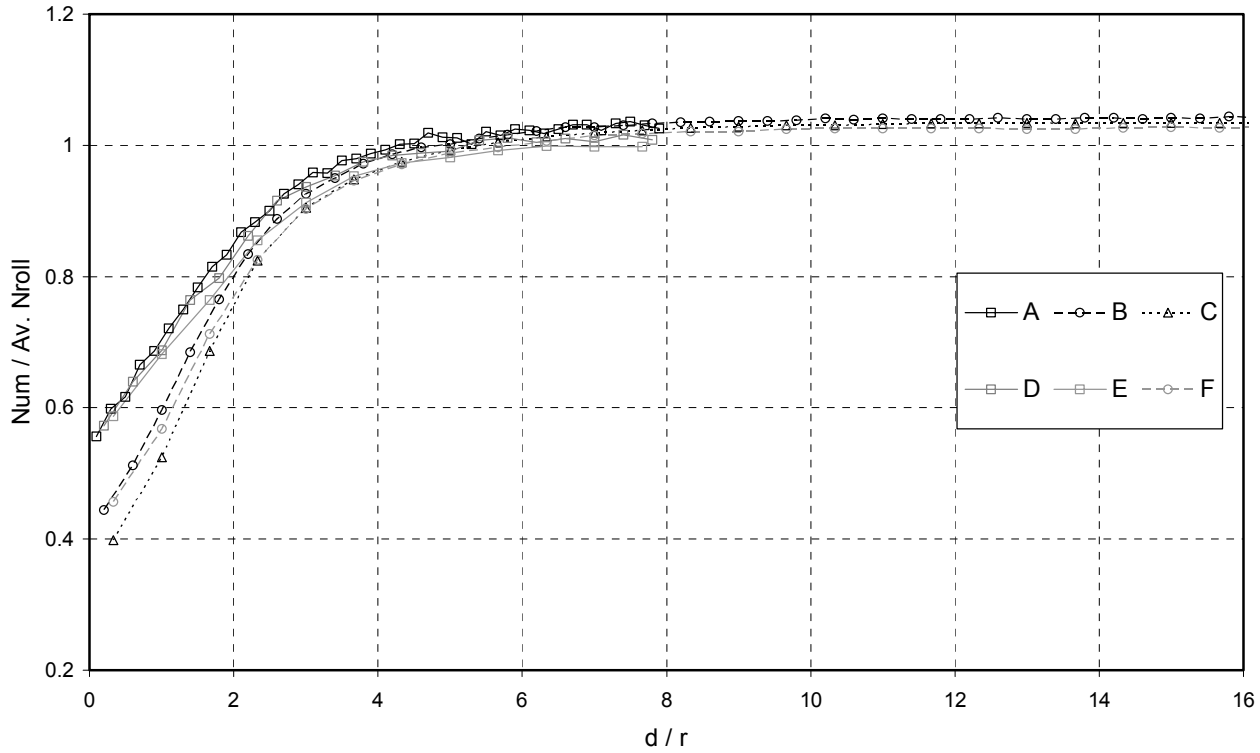

Figure 7: Dependence of the number of placed spheres (Num) on d

Figure 7 shows that, after making the correct normalizations, the relationship between number of placed spheres (which also means solid ratio) and *d* is the same for all 6 analysis, provided d/r is large. It represents, therefore, a general rule for packings obtained by subsequent deposition, and can be used in this research in order to produce the necessary different configurations.

However, we can note that the "roll-down" algorithm (that provides Av. Nroll) gives a slightly looser packing than the algorithm of Figure 6 with large *d.* Considering Figure 6, the "roll-down" algorithm would give the central result and not the right-hand one. Thus the maximum ratio in Figure 7 is slightly greater than 1, while a ratio of 1 is observed for d/r = 5 ± 1.

The variability presented in Figure 7 for low d/r values is due to the first layer of placed spheres, i.e. the bottom of the packings: all the packings, in fact, have to start with a similar first layer, which for low values of d/r is denser than subsequent layers of spheres placed. This denser region affects the result in different proportion as the total number of spheres in the assembly changes. A, D and E, which have similar Av. Nroll, are affected more than B and F that, again, are affected more than C. Anyway, this imprecision will disappear from the real tests results when the bottom, top and side spheres are discounted as atypical and only the internal ones will be considered.

Solid Ratio evaluation

The solid ratio (SR) of the Voronoi cell and of the whole assembly has been used to represent the packing degree throughout all this work. It is generally calculated as the ratio between the solid part and the total volume (2)

$$SR = Vsolid/Vtotal \quad (2)$$

Voronoi cell determination

Receiving as an input the Cartesian coordinates of the spheres' centres, Matlab software [9] is able to find the coordinates of the vertices of each Voronoi cell within the given packing. Knowing these vertices, the Voronoi cell is the only convex solid that they can form. To calculate its volume, the triangular faces of this solid were determined using the Matlab function "convhulln", which finds all the different "triplets" of vertices that form the convex solid's faces. Once these triplets are known, the Voronoi cell's volume is found as the sum of the volumes of the tetrahedrons that each triangular face forms with the cell's centre (the centre of the central sphere).

MAIN RESULTS

Results from the spheres generation

As shown in Figure 8, all of these final configurations have a minimum coordination number of 6, which means that this is the minimum number of spheres needed to randomly occupy the whole available surface. Every random sphere generation has, therefore, reached at least 6 spheres placed around a central sphere, while only one of them was found to reach 12 (the maximum value as predicted by Kepler [8]).

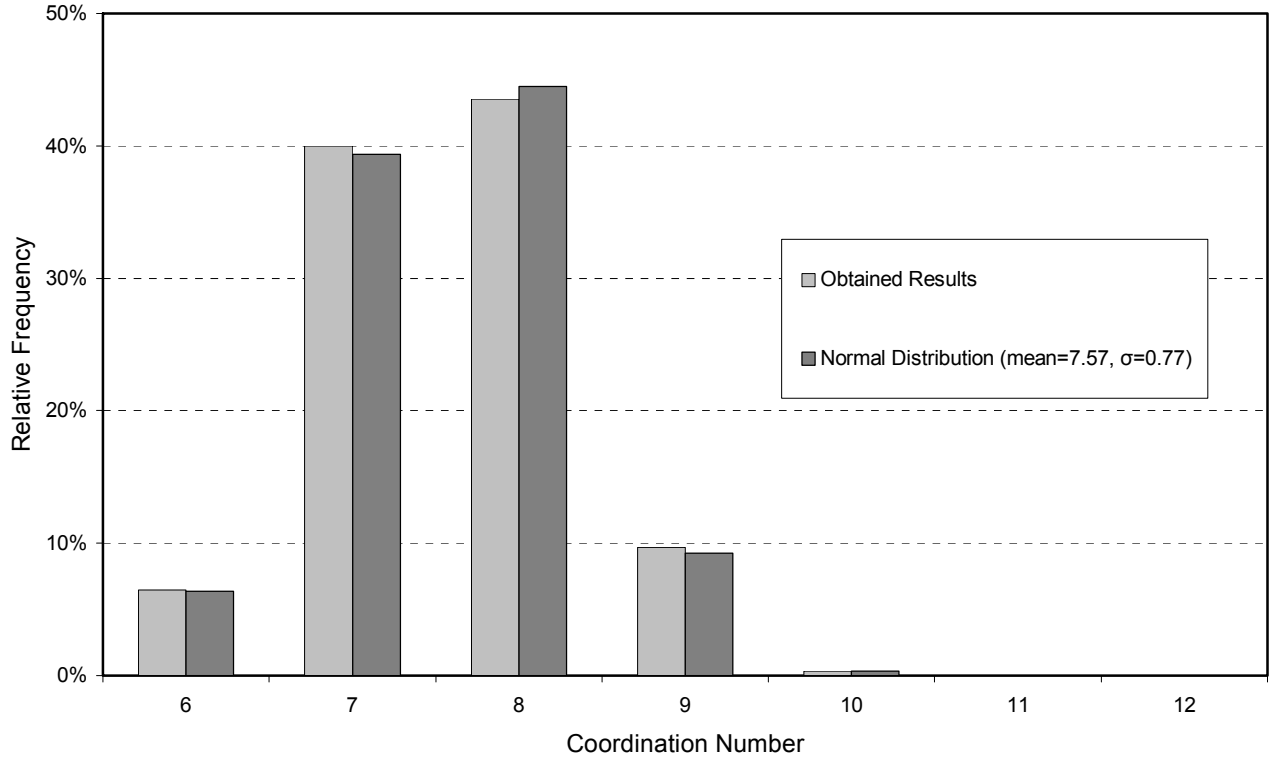

Figure 8: Relative frequencies of the different final coordination numbers

It can be noted from Figure 8 that the relative frequency of the number of spheres needed to completely occupy the surface of an identical sized sphere follows a normal distribution with mean value = 7.57 and standard deviation = 0.77. It has been found that the relative frequency of coordination number also takes a normal distribution when the outer spheres are of different diameter to the central sphere but, even if considered by the authors an interesting point of discussion, this will not be referred to further in this paper for reasons of clarity and brevity.

Of course, each final configuration of N spheres may also be considered as producing an intermediate configuration for each n < N spheres group, consisting in the right number of spheres in chronological order of deposition. For analytical convenience (discussed later) only assemblages having 5 or more spheres (i.e. 4 or more placed around the central sphere) are considered in this paper. A 9-spheres configuration (coordination number = 8) will, then, produce one interim configuration for each of the 5, 6, 7 and 8 spheres

groups considering, respectively, the first 4, 5, 6 and 7 placed spheres. The total number of configurations produced is, thereby, approximately 370000.

This kind of configuration does not consider all those situations where a sphere is not touching the central one but is close enough to influence its Voronoi cell (Figure 9a is considered while Figure 9b should have been).

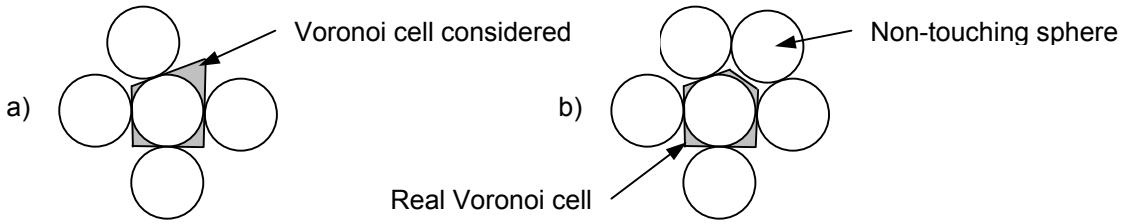

Figure 9: Influence of non-touching spheres on the Voronoi cell

Investigating these configurations to find the link between solid ratio and coordination number is, therefore, useless for the purpose of predicting the properties of a spheres' assembly, but nonetheless an analysis has been performed thinking that its results may find their applications in other research. From this point of view, the main result is given in Figure 10.

Moreover, in this analysis is not possible to calculate the solid ratio for coordination numbers less than 4, as in those cases the Voronoi cell is "open" (there can't be any solid with less than 4 faces), and this is why in Figure 10 the coordination numbers start from 4. As will be shown later in the results from the second method, in reality particles with coordination number less than 4 can still have a closed Voronoi cell because, being inside the assembly, they will be surrounded by other particles, even without being touched.

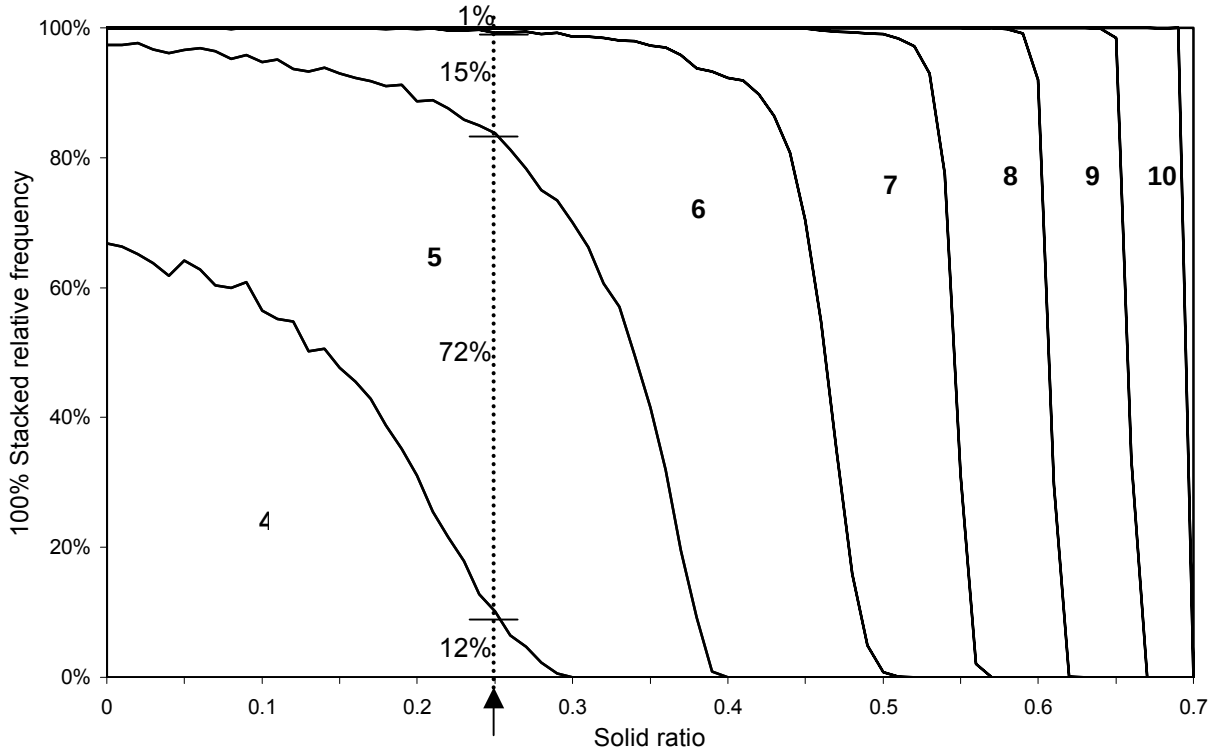

Figure 10: Stacked relative frequencies of coordination numbers against solid ratio (Method 1)

Figure 10 is meant to be read in the following way: for a given solid ratio, a vertical line is divided by the chart in segments that are proportional to the relative frequency of each coordination number. For example, for a solid ratio of 0.25 the distribution of coordination numbers is summarized in Tab 2.

Tab 2: Numerical example of Figure 10 for SR = 0.25

Coordination number	Relative frequency
4	12%
5	72%
6	15%
7	1%

For each value of coordination number, the number of configurations produced is such that it is possible to derive a statistic of the outer spheres distribution on the central sphere's surface. The volume of the Voronoi cell (Vv) formed can represent a measure of this distribution: a uniform configuration will have a lower Vv than a less uniform one. In particular, unstable configurations (that is where the Voronoi cell is open-ended – see Figure 11c) will have Vv = ∞.

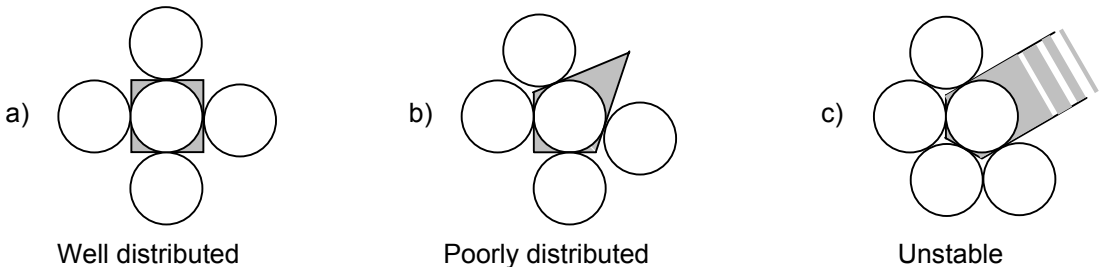

Figure 11: Influence of the outer spheres' distribution on Voronoi cell volume

For example, with a coordination number of 6 the best distribution corresponds to the situation where the Voronoi cell is a cube (Figure 2 illustrates this while Figure 11 shows the variation, in a 2 dimensional sketch, of the increase of the Voronoi cell volume when four spheres are poorly distributed around the central sphere). The volume of this cube is also the minimum volume (Vvmin) that a Voronoi cell can have if formed by only 6 spheres. Any distribution of the 6 spheres which differs from this one will present a larger value of Vv, and this value will increase as the distribution gets less uniform.

Based on these considerations, the concept of "contact distribution" (D) of a particle can be introduced by the following definition (2):

$$D = Vvmin/Vv \quad (3)$$

Obviously, Vvmin is a function of coordination number. The normalization of Vv by Vvmin makes this concept independent of a sphere's radius (as this also affects the Voronoi cell volume) and from coordination number: a configuration of 4 spheres (or 4 contacts) uniformly distributed is, therefore, considered as well distributed as a configuration of 12 spheres uniformly distributed, being in both cases D = 1.

Note that Vvmin for a coordination number of 3 is always ∞ (as there can not be any solid with less than 4 faces) and it is for this reason, therefore, that only coordination numbers greater than 3 have been considered in this paper. Tab 3 shows the values of Vvmin that were found for the different coordination numbers and that were used for the subsequent analysis.

Tab 3: Value of Vvmin for each coordination number (spheres' radius = 1)

Coordination number	Obtained Vvmin
4	13.91
5	10.50
6	8.12
7	7.33
8	6.75
9	6.30
10	6.02
11	5.85
12	5.56

An analytical value of Vvmin can be found for those coordination numbers whose minimum Voronoi cell is a regular polyhedron, i.e. 4 (tetrahedron), 6 (cube) and 12 (dodecahedron). These analytical values can be calculated by equations (4), (5) and (6) and are given in Tab 4 [11].

Tab 4: Vvmin for regular polyhedra with central sphere radius of 1

Coordination number	Analytical Vvmin
4	13.86
6	8.00
12	5.55

$$\theta = acos[(cos\alpha - cos^2\alpha) / sin^2\alpha] \quad (4)$$

$$s = ri * 2 * tan(\pi/n) / [(1-cos\theta)/(1+cos\theta)]^{1/2} \quad (5)$$

	Tetrahedron	Cube	Dodecahedron	
Volume =	$2^{1/2} * s^3 / 12$	s^3	$(15+7*5^{1/2}) * s^3 / 4$	(6)

where α is the plane angle between two consecutive sides, θ is the dihedral angle between two faces, n is the number of sides in each face, ri is the radius (ri = 1 in our case) and s is the side length.

As can be seen comparing the data from Table 3 and Table 4, the minimum Voronoi cell volumes obtained are entirely consistent with the analytical results. In particular, they provide upper bound values of the analytical solutions, showing that all the configurations generated respect these minima. Therefore, it is reasonable to assume that this method is also indicating reliable values of the minimum Voronoi cell sizes when no analytical solution is available.

Figure 12 shows the cumulative frequency of D (Equation 3) for each coordination number. For a given value of D, say D*, this chart shows the percentage of spheres with a given coordination number that were found to have D<D*. A numerical example is given in Tab 5.

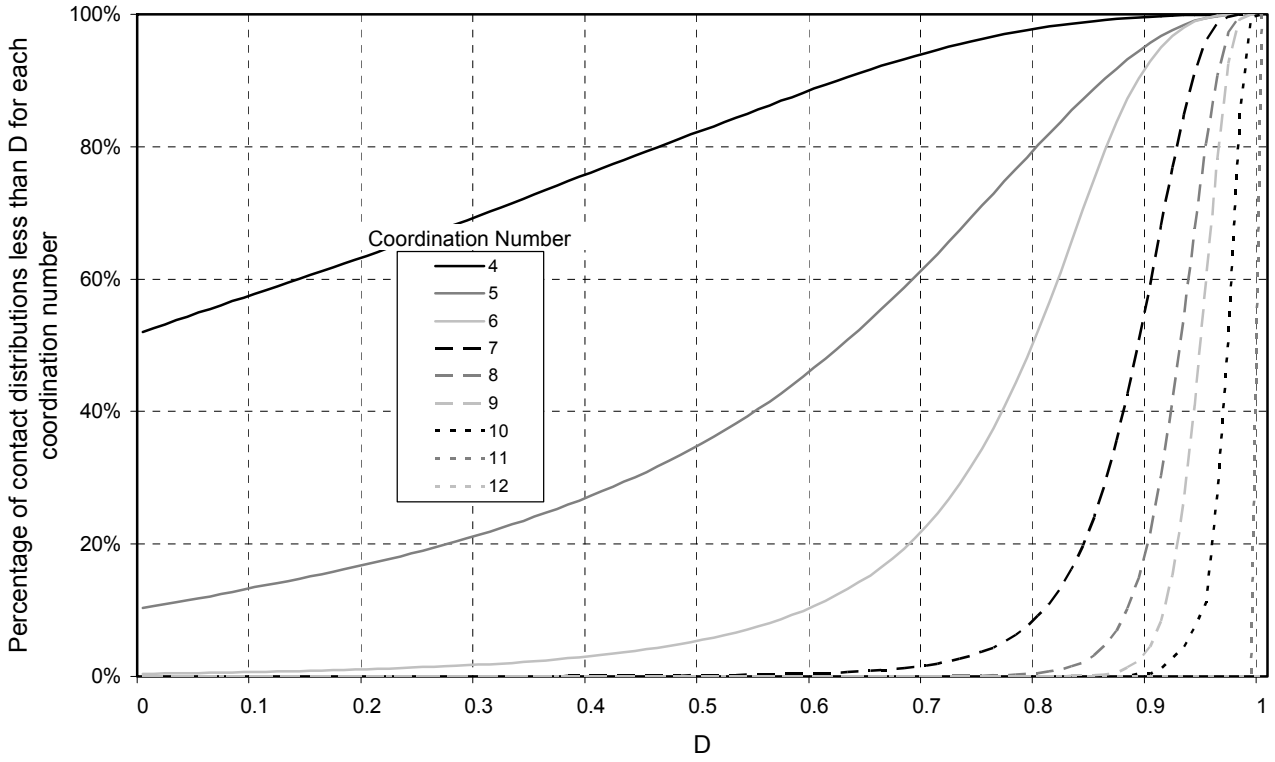

Figure 12: Cumulative frequencies of contact distribution (D)

Tab 5: Numerical example of Figure 12 for D = D* = 0.4

Coordination number	% of spheres with D<D*
4	76
5	27
6	3

In theory, the maximum coordination number for an unstable particle (i.e. Vv = ∞ → D = 0) is 9. Consider a configuration such as the face-centred cubic, which has 6 spheres along an equator of the central sphere and 3 at the top and bottom (for a total coordination number of 12), it is possible to see that an open-ended Voronoi cell is obtained subtracting the 3 top or bottom spheres, leaving a coordination number of 9. However, it can be seen from Figure 12 that, in reality, unstable spheres are very unlikely to be generated with a coordination number higher than 6. This is anticipated as, according to Kepler's conjecture [8], 12 is the maximum possible coordination number, so 6 is the expected maximum number of spheres that can be randomly placed in one hemisphere yet leave the other open-ended such that Vv = ∞. The 7^{th} sphere would be expected to be placed in the opposite hemisphere and thus to stabilize the particle.

The likelihood of an unstable arrangement with 7, 8 or 9 spheres around a central one can be evaluated noting that it represents a very narrow subgroup of the 11, 12 and 13-sphere groups. Intuitively, we can say that the situation of placing the first 7, 8 or 9 spheres in the same hemisphere is much more likely to have happened for the 13-sphere group (coordination number = 12) than for the 11-sphere group (coordination number = 10) because with lower final coordination numbers the spheres are less well packed, therefore we can deduce that the probability of an unstable Voronoi cell with coordination number of 7, 8 or 9 is highest for a final coordination number of 12, which, on the other hand, has the lowest frequency occurrence. The probability of the first 9 outer spheres of a 13-sphere assembly forming an unstable configuration can be calculated as follows.

Given a group of 12 outer spheres, we are selecting 9 of them. The total number of ordered combinations of 9 elements out of 12 is

N (9/12 ordered) = 12! / (12-9)!

Therefore each 9-element group has a probability of

P (9/12 ordered) = (12-9)! / 12!

The acceptable combinations are those comprising the first 9 elements placed, although they may be selected in any order. Their number is

N (9/9 ordered) = 9!

Therefore the probability for the first 9 spheres to be the ones we choose from a final placing of 12 around a central sphere is

*N (9/9 ordered) * P (9/12 ordered) = 9! * (12-9)! / 12! = 3! / (12*11*10) ≈ 0.0045 = 0.45%*

Finally, considering that we can choose the 9 spheres in 8 different ways, the indicated probability is then

*P (unstable) = 8 * 9! * (12-9)! / 12! = 8 * 3! / (12*11*10) ≈ 0.0364 = 3.64%*

Thus, this is the probability for a final 13-sphere group to produce an interim unstable 10-sphere group. For the reasons explained before, we can expect this percentage to be much lower when the coordination number is 11 and 10. Considering that these percentages must also be multiplied by the respective coordination number's relative frequency, these observations fully explain the results shown in Tab 6.

Tab 6: Number of unstable configurations for each coordination number

Total number of spheres	Coordination number	Inspected Configurations	Unstable Configurations	%	Instability
4	3	80270	80270	100.00	Certain
5	4	80270	41744	52.00	Possible
6	5	80270	8317	10.36	Possible
7	6	80270	313	0.39	Unlikely
8	7	75094	1	0.00	Very unlikely
9	8	42973	0	0.00	Very unlikely
10	9	8027	0	0.00	Very unlikely
11	10	265	0	0.00	Impossible
12	11	12	0	0.00	Impossible
13	12	1	0	0.00	Impossible
TOTAL		367182			

Stated another way, it is reasonable to assume that an 8-sphere arrangement (a central sphere plus 7 added) or a 9, 10, 11, 12 or 13-sphere arrangement is inherently stable. Moreover, 52% and 10% of all the possible configurations of particles with coordination numbers respectively of 4 and 5 are unstable, which means that, in an assembly subjected to external forces, they would not take part in the global mechanism. This aspect is of major importance when trying to relate aggregate mechanical properties to particle arrangement, and will, therefore, need further investigation than has been possible in this paper.

Results from the second method

The box-filling algorithm has been used gradually varying the parameter *d* in order to obtain different packing degrees as explained earlier in this paper. As can be seen from Figure 7, the linear increase of *d* does not lead to a linear increase in solid ratio. As d increases, solid ratio reaches its maximum after which it remains constant. The use of this algorithm brings, therefore, to an uneven distribution of solid ratios through the whole range, with the number of dense packings larger than the number of loose ones. To obtain a uniform set of data, i.e. a number of results regularly distributed, the results have been grouped by solid ratio and their coordination number frequencies have been averaged within each group (defined as the stated solid ratio ± 0.025). Figure 13 shows the resultant data.

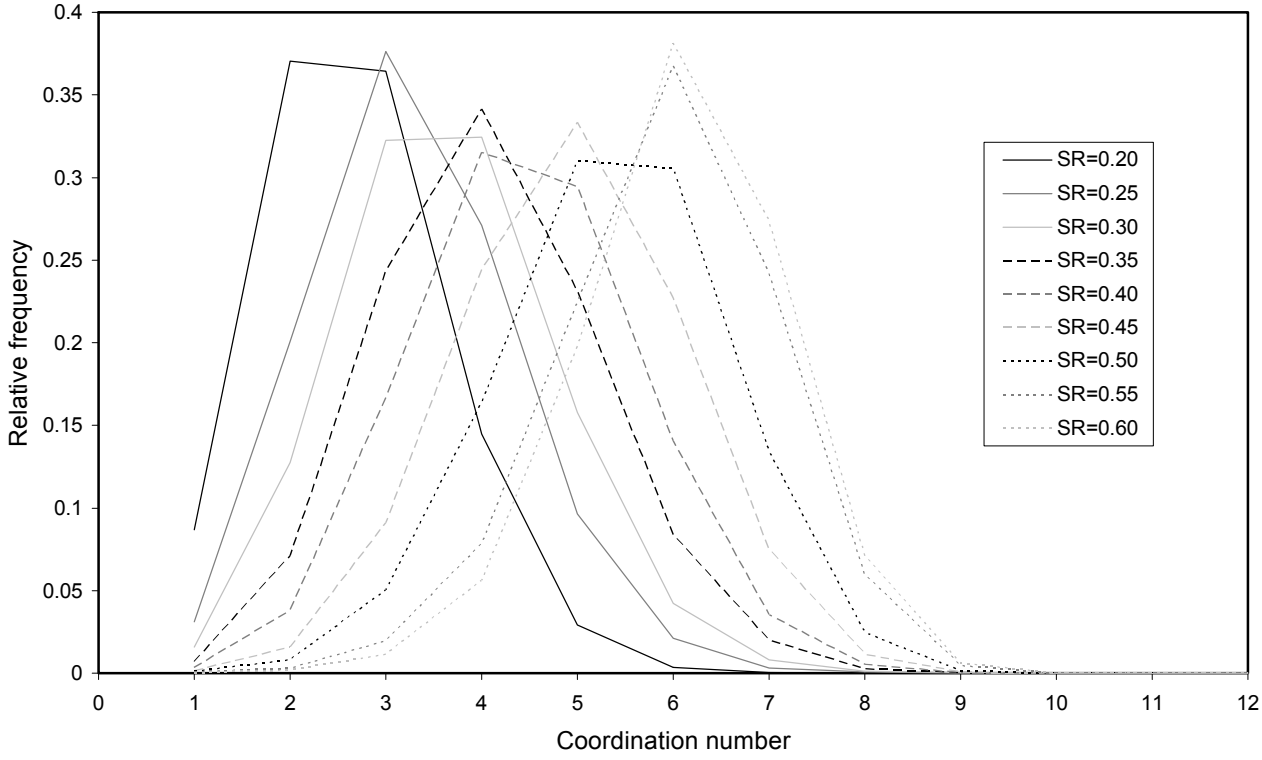

Figure 13: Relative frequencies of coordination number for solid ratio from 0.20 to 0.60

As already observed by M. Oda [6], who obtained similar curves by physical experimentation, these curves are very close to normal distributions, therefore is possible to describe them by means of their average value (AvCN) and standard deviation (StD). Figures 14 and 15 show these parameters for the distributions in Figure 13.

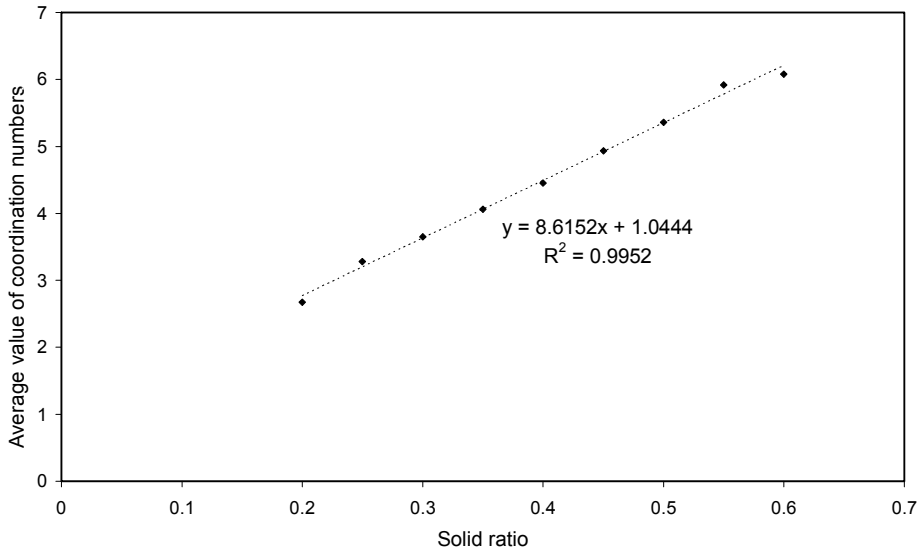

Figure 14: Average coordination number for solid ratio from 0.20 to 0.60

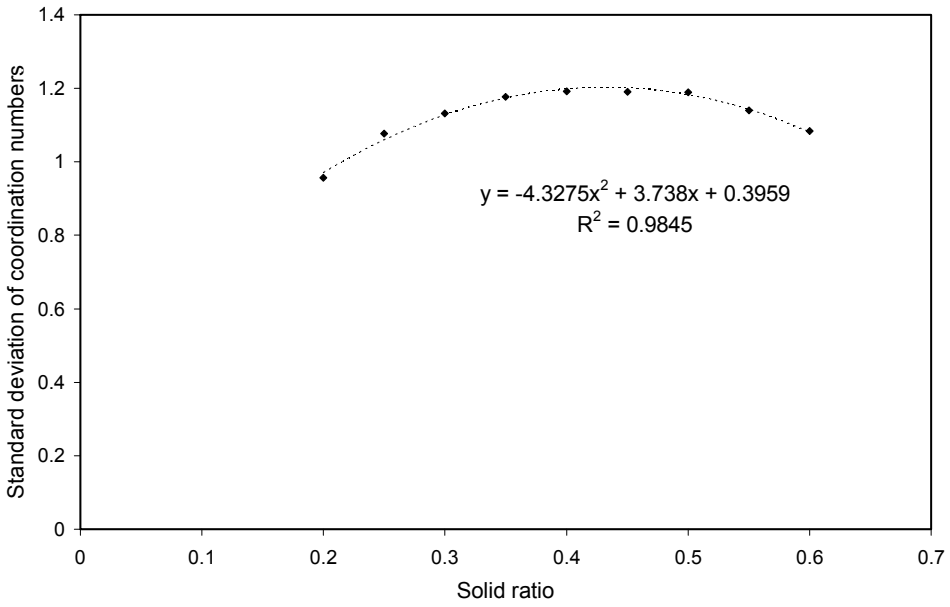

Figure 15: Coordination number's standard deviation for solid ratio from 0.20 to 0.60

The two sets of data present well-defined trends when plotted against solid ratio, therefore it is possible to suggest the two equations that fit them best ((7) and (8)) as suitable for the purpose of this research.

*AvCN = 8.6152*SR +1.0444* (7)

*StD = -4.3275*SR^2 +3.738*SR +0.3959* (8)

Equations (7) and (8) have also been used to produce the chart in Figure 16, which should be read in the same way as Figure 10 for the first method.

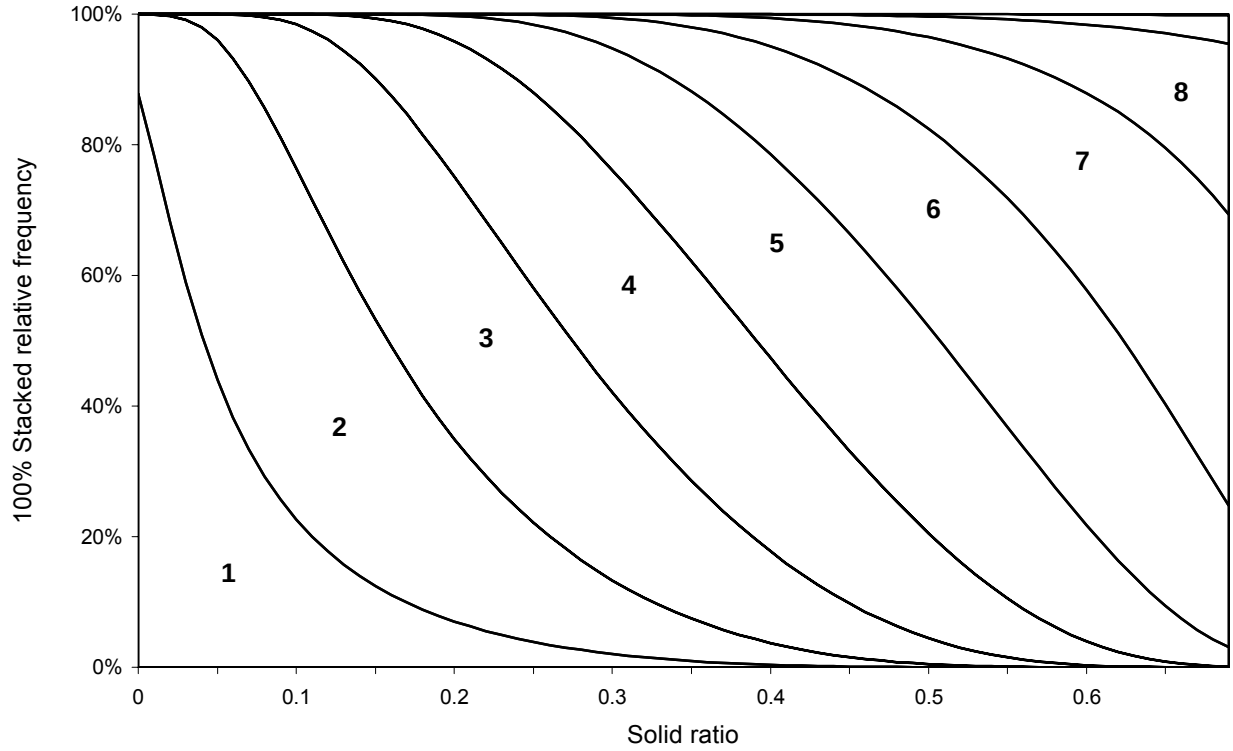

Figure 16: Stacked relative frequencies of coordination number against solid ratio (Method 2)

CONCLUSION

The aim of the study presented in this paper was to investigate the properties of equal spheres assemblies from the geometric point of view as a pre-cursor to investigating effects of packing on aggregate properties. The understanding of spatial characteristics of single-size sphere arrangements is the fundamental part of a more general packing theory for unbound granular materials, which has been conceived to explain particles' micro-mechanics. In particular, as evidenced by previous research, attention must be focused on particle coordination number, which is the number of contact points that each particle has with its neighbours.

Two methods have been used to generate large numbers of random sphere configurations from which to derive statistical observations: random placement of spheres on an equal size sphere's surface and random box filling with equal spheres. Basically, the first method only considered the relationship that occurs between one sphere and its touching neighbours, while the second one simulated large sphere assemblies analysing their global arrangements. Therefore, being two very different approaches, they have led to consideration of different aspects of the subject.

As a first approach, an algorithm was developed that has proved to be suitable for generating a large number of configurations of spheres around a central one. The analysis of these results provided important information about the contact points' distribution on the central particle surface. The concept of "contact distribution" (D) is introduced in equation (3) by means of the Voronoi cell volume. This parameter is suitable to describe the contact points' dispersion and, therefore, its statistical distribution for the different coordination numbers has been analysed. The results obtained show that 52% and 10% of spheres with coordination numbers respectively of 4 and 5 were found to have an "unstable" contact points' configuration (see Figure 12). They also reveal that unstable arrangements are only likely to appear with 7 or less spheres (coordination number ≤ 6), in line with a logical extension of Kepler's observation.

The second method has proved to be the best way to accomplish the main target of this study, i.e. to develop a tool to predict the distribution of coordination number as a function of packing degree in equal size sphere assemblies. The introduction of the parameter *d* in the algorithm allowed the investigation of the desired range of solid ratios. The results obtained prove that, for any solid ratio, the coordination number follows a normal distribution that can be predicted using equations (7) and (8) developed herein.

Where analytical solutions of physical modelling results are available, we have shown that the work described delivers the same results. The advantage of this new approach is that the statistical variability has also been defined revealing the likelihood of the known solutions being realised in practice.

Finally, it must be said that, aside from the main results, a number of interesting observations can be made that have not been fully developed in this paper for reasons of clarity. Due to the width of the topic, some of them may find a place in the authors' future work about unbound granular materials mechanics, some others may be of interest for studies in powder mechanics, material science, etc.

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