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Collective random packing of disks in a plane under the influence of a weak central force

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Abstract. Some special effects in a 2D or 3D packing appear when this packing is made with particles belonging to an initially dense system. In order to achieve a better understanding of 'arching effects', a computer simulation of the collective random packing of disks in a plane under the influence of a weak central force has been set up. This work can be regarded as the first approach to the modelling of actual granular stackings resulting from mixing, pouring or fluidising particles. The dependence of the final packing fraction and mean coordination number on the initial density and on the step length has been studied on stackings of uniform disks. These functions can reach values as low as 0.76 and 3.40.

1. Introduction

Some particular collective effects can be observed in 2D or 3D real packings. To understand the phenomena and to control these effects a 2D simulation has been carried out. This work will be described and the main results analysed after a review of the literature.

Clarke and Wiley (1987) distinguish two types of method for preparing hard-sphere packings on a computer: the sequential addition model and the collective rearrangement model.

The first method starts with a seed cluster and brings in additional spheres, one at a time, placing each one under the action of a central or vertical force until a mechanical equilibrium position is reached. Whenever the starting position of a sphere is randomly chosen, a reference packing is obtained: 'random packing built grain by grain'. Such a packing has the following characteristics: the packing fraction C is about 0.58–0.59, and the mean coordination number z is 6 (Powell 1980, Tory *et al* 1968, 1973, Visscher and Bolsterli 1972). The z-value is imposed by the building mode: to remain in equilibrium under gravity each sphere is lying on three contacts; the total number of contacts N_c in a packing of N equal spheres is $3N$. Since the number of particle pairs which is $\frac{1}{2}zN$, is equal to N_c, the value of z is 6.

The real packing closest to the reference packing is the so-called 'loose random packing' obtained by pouring the particles slowly into a receptacle from a small fall height. The range of packing fractions of this packing is 0.59–0.60 (Scott 1960, Bernal and Mason 1960, Macrae and Gray 1961) and z is about 6 (Bernal and Mason 1960). Nevertheless some important differences are to be noted; the frequency of coordination

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numbers and the pore size distribution function are larger in the actual packing than in the simulated packing (Tory *et al* 1968, 1973). Two phenomena can explain this fact.

(i) On the one hand, a ball falling to the surface of the experimental sphere packing changes its kinetic energy into vibrations when the collision occurs. These vibrations can lead to rearrangements in the superficial layers.

(ii) On the other hand, if the density of the falling balls is high enough, the spheres are not placed one by one; several particles can be locked together so that an arch can be formed. Bernal and Mason (1960) have pointed out that large cavities can be observed in loose packings of spheres. These holes are larger than the five canonic polyedra established by Bernal (1960). Meldau and Stach (1934) too observed some arches on sections of loose packing of spheres.

In the collective rearrangement model, the positions of the spheres are randomly chosen. Then the sphere radius is increased step by step. At each step, the centres of two overlapping particles are kept apart along the direction of the straight line joining them. This process is repeated until the overlap-free packing fractions converge. Reducing some sphere radii and vibrating the spheres unlocks the particles and a 'close random packing' with $C = 0.64$ and $z = 6$ is obtained (Clarke and Wiley 1987, Jodrey and Tory 1981).

These characteristics are in fairly good agreement with those of experimental packings obtained after compression and vibration of loose random packings. Several experiments have shown that a packing fraction equal to 0.64 is a maximum value for random packings. Larger values can be reached by means of intense and long vibrations (Debbas and Rumpf 1966) or shear stresses (Scott *et al* 1964, Rutgers 1962), but in both cases long-range order occurs.

All the simulations performed up to now are not adapted to a description of packings of grains obtained after particle processing such as mixing. The models do not take into account either the percussion of the falling balls or collective interactions between grains. Macrae and Gray (1961) have clearly shown the important effect of these two phenomena. They poured spherical particles into a receptacle and made the particles flow rates vary; evidence of the influence of the falling-sphere density C_0 was obtained:

(i) When C_0 is small, the packing fraction C of the resulting packing is that of the loose random packing (0.595 ± 0.005).

(ii) When C_0 becomes higher, the kinetic energy of falling particles allows the spheres in the upper layers of the packing to be rearranged into configurations which are more stable mechanically; the packing fraction increases.

(ii) For the highest C_0 values, the rearrangements become impossible because the spheres are locked together when arriving at the surface, and the packing fraction decreases again.

Macrae and Gray also observed that, for the higher velocity of spheres obtained with a higher fall height, the packing fraction increase was larger. On the contrary, for systems in which the velocity is weak and the initial density large enough, collective assemblies of spheres with arching effects must prevail. In fact, this is observed in fluidised beds of spheres when the flow rate is reduced to zero (C becomes less than 0.58; Wakeman 1975) and similarly when a vessel containing a packing of spheres is placed upside down (Epstein and Young 1962). Undoubtedly these phenomena also play a role during mixing. For fine particles, these phenomena are very important because the arches offer a higher mechanical stability due to stronger intergranular bondings. In the same way,

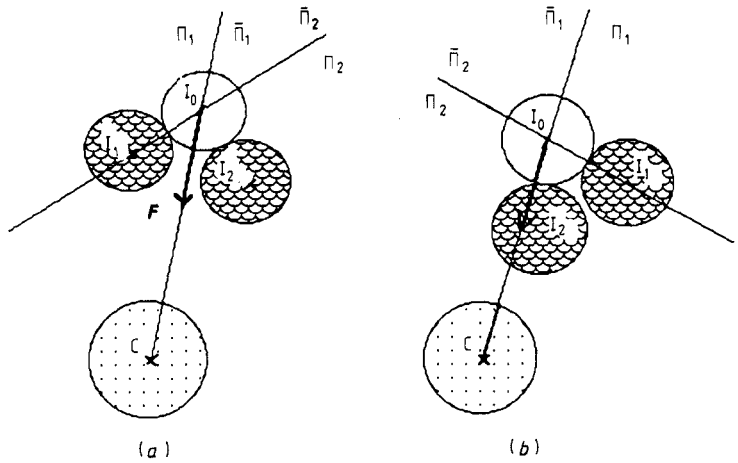

Figure 1. Condition for the rotation of a moving disk: (*a*) locked disk $\Leftrightarrow I_2 \in \Pi_1 \cap \Pi_2$; (*b*) the rotation is allowed.

if particles are polyhedral, face-to-face contacts give the arches a greater stability. Ammi *et al* (1987) have shown that the minimum packing fraction of 2D polygon packings was obtained with pentagons and was as low as 0.78 (to be compared with about 0.82 for disks).

2. Algorithm to prepare a collective 2D packing

The present work explores a numerical method for preparing grain packings in which collective effects are simulated on a computer. Because of the complexity of the phenomena we have been dealing with a 2D space. Disks are moved collectively under the influence of a weak central force; the percussion effects will be neglected, which corresponds to the physical case where the particles have a low velocity. Under such conditions, arches can be obtained. In spite of their low mechanical stability, they will never be destroyed afterwards, and the characteristic features of random packings with a low packing fraction can be seen.

We have simulated a collective random packing of N equal disks under a central force on an M380 Olivetti computer. First of all, a disk is placed in the centre of the plane. This disk (radius R_0) is slightly larger than all the others (radius R) to avoid the formation of hexagonal structures. N randomly chosen disks are then located in a great circle, the radius ρ of which is a function of N, R and the fixed initial density C_0:

$$\rho = \sqrt{NR^2/C_0}.$$

The program consists of a series of cycles. At each cycle, all the disks are moved, one by one. The order of displacement corresponds to the order of the distances to the centre at the beginning of the cycle (nearest disks being moved first). Each disk is moved toward the centre with a step length p small enough that each cycle on the N particles simulates a slight collective motion of the disk assembly. If a disk I_0 happens to encounter another disk I_1 during its straight movement, then it is assumed that the target disk I_1 does not move. The disk I_0 rolls around I_1. During the rotation, if a collision with a second disk I_2 occurs, two criteria are investigated (figure 1).

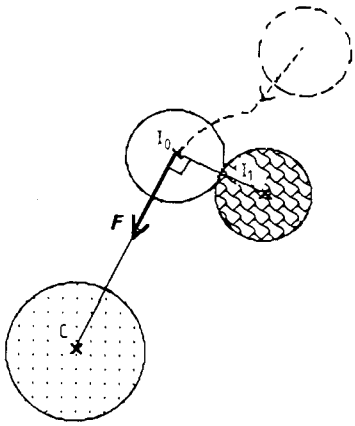

Figure 2. End of the rotation of a disk.

(i) The two target disks block the moving disk I_0 (figure 1(*a*)). Then I_0 is stopped and the following disk is considered.

(ii) I_0 can roll on the second disk under the action of the central force (figure 1(*b*)). Then it continues.

A simple geometrical test on the respective positions of I_2 and the half-planes Π_1 limited by the straight line I_0C and containing I_1, and Π_2 limited by the straight line I_0I_1 and containing C allows us to choose between these two cases.

After the target disk has been passed, the rotating disk can recover its rectilinear motion towards the centre (figure 2). The movement is stopped when one of the three following conditions is achieved.

(i) The moving disk encounters the central disk.

(ii) The configuration in figure 1(*a*) is obtained.

(iii) The length of the total displacement of the centre of the moving disk (rectilinear and curvilinear) is equal to the step p.

Then the following disk is examined and, when all the disks have been treated, a new cycle starts. The program stops when no disk is moved during a cycle; the packing is then in equilibrium under the central force.

3. Results

The program written in PASCAL 4.0 is capable of handling approximately 1500 disks. In general, 500 disks are sufficient to give consistent characteristics. The dependence of the properties of the final packing upon the step length p and the initial density C_0 has been examined on packings of 500 disks. The same principle is adopted to measure packing fraction and coordination number. The packing is cut in circular 'rings' which are $R/2$ thick. The first ring lies around the central disk. Measurements are performed for each ring, and the curve of variation in the parameter considered is drawn as a function of the distance to the centre. The average is evaluated after elimination of the

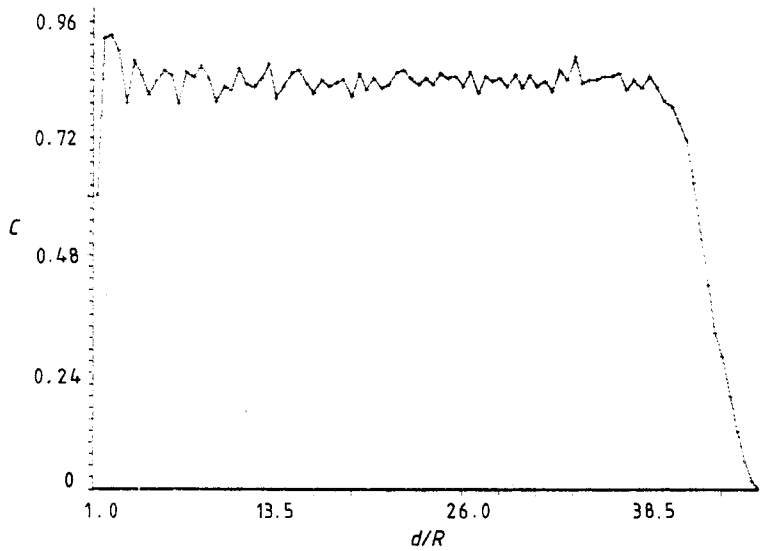

Figure 3. Packing fraction as a function of the relative distance to the centre ($C_0 = 0.1p/R = 200$).

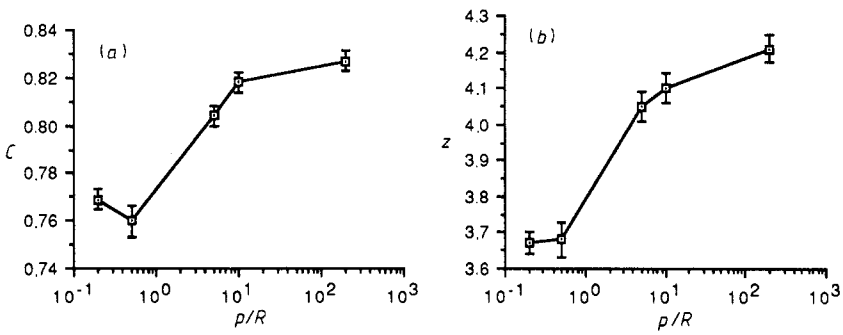

Figure 4. Development of (*a*) packing fraction and (*b*) mean coordination number versus relative step length for $C_0 = 0.1$

central area and the edge of the packing (figure 3). So as to estimate the packing fraction in a ring, we first determine the disks intersecting the ring. The area A_s of the surface cut by these disks in the circular ring is calculated according to the method explained in the appendix. The packing fraction in the ring is given by A_s/A_c where A_c is the ring area. To measure the mean coordination number, we must look for the disks i whose centres are within the ring. All the disks j for which $d_{ij} < 2R + 10^{-7}$ are counted for every disk i (d_{ij} is the distance between the centres of i and j). We average the values obtained for all the disks i and thus obtain the mean coordination number in the ring.

Figures 4(*a*) and 4(*b*) show the influence of the step length on the packing fraction and the average coordination number z, respectively, for an initial density $C_0 = 0.1$. *When p is larger than the great circle radius* ρ used in the initial drawing lots, the disks will move one by one and each of them will find a definitive location immediately at the

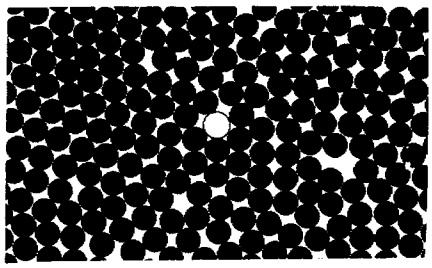

Figure 5. Packing with $C_0 = 0.1$ and $p/R = 200$.

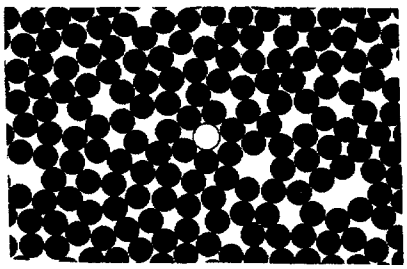

Figure 6. Packing with $C_0 = 0.1$ and $p/R = 0.2$.

first cycle. Then *a random packing built 'grain by grain' has been simulated*. In this case some regions present a kind of hexagonal order (figure 5). The packing fraction and mean coordination number can vary considerably. Therefore, mean values have been calculated from several packings of 1500 disks: $C \simeq 0.835 \pm 0.005$ and $z = 4.21 \pm 0.05$. By contrast, using a small value for the step length with respect to the grain size allows us to simulate collective displacements of disks. Figure 4 indicates that no important changes in the results can be noted when p/R-values are less than or equal to 0.5. So *$p/R < 0.51$ can be used to simulate collective random packing* (lower values strongly reduce the program's rate). In this case, a '500 equal-disks run' takes approximately 2 h (CPU time). Figure 6 represents this packing with some arches. C and z strongly depend on the initial density.

The variation in the initial density over a wide range (10^{-3}–0.5) allows us to study the associated changes in packing fraction and mean coordination number for packings built collectively ($p/R = 0.5$) (figure 7). For C_0 less than 10^{-3}, the number of cycles to achieve the packing is so large that the run time exceeds several days. For $C_0 > 0.5$ it is impossible to assign locations to the N disks in the initial circle of drawing lots (radius ρ fixed). When C_0 is small, collisions between disks during the stacking process are rare and the packing has the characteristics of a 'grain-by-grain' nature although it is built collectively (for $C_0 = 10^{-3}$, $C = 0.822 \pm 0.003$ and $z = 4.15 \pm 0.05$). Crystallised regions may be encountered. The minimum packing fraction is expected to be at a high starting concentration, where the collective effects become very important. This expectation is fulfilled but the changes are surprisingly significant. For $C_0 \rightarrow 0.5$, $C = 0.756 \pm 0.003$ and $z = 3.40 \pm 0.02$. Zones presenting hexagonal order do not exist (figure 8). Another difference between the 'grain-by-grain' packing and the collective packing with minimum packing fraction can also be pointed out in the distribution of

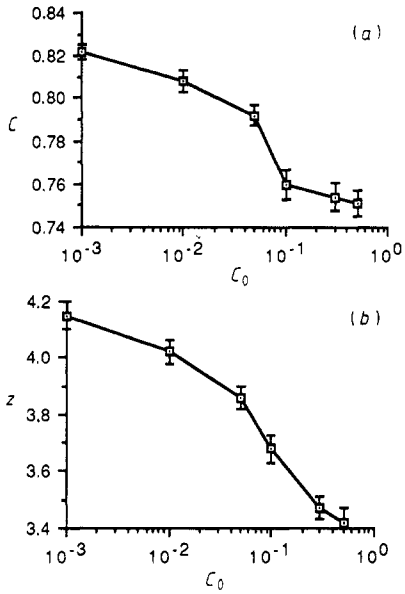

Figure 7. Development of (*a*) packing fraction and (*b*) mean coordination number versus initial density ($p = R/2$).

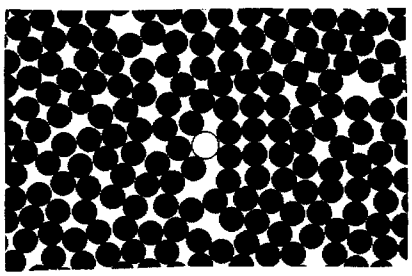

Figure 8. Packing with $C_0 = 0.5$ and $p/R = 0.2$.

coordination numbers. This distribution has been calculated after elimination of the central area and edge of the packing. In the 'grain-by-grain' packing, disks are not able to have a coordination number lower than 3, and the fraction of disks having a coordination number of 4 is very high (figure 9). In collective packings, the number of disks having a coordination number of 4 or 5 is not so important and some disks have a coordination number of 2, which is relevant to the packing mode (figure 10).

4. Discussion

It seems interesting to compare our results with those published in other papers dealing with 2D packings. Two theoretical independent calculations lead to the same estimation of the packing fraction in random disks packings; Bideau *et al* (1986) give $C = \pi^2/12 = 0.822$, and Berryman (1983) gives $C = 0.823 \pm 0.02$. Laboratory experiments and 'grain-by-grain' simulated packings have produced packing fractions between 0.82 and

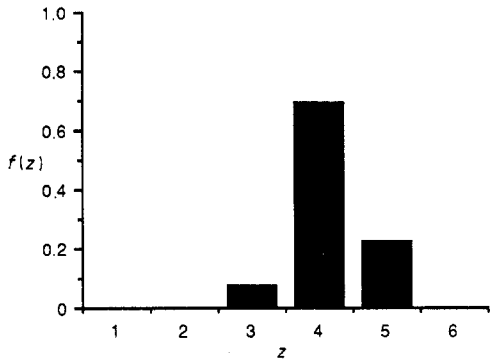

Figure 9. Distribution of coordination numbers ($C_0 = 0.001 - p/R = 2500$).

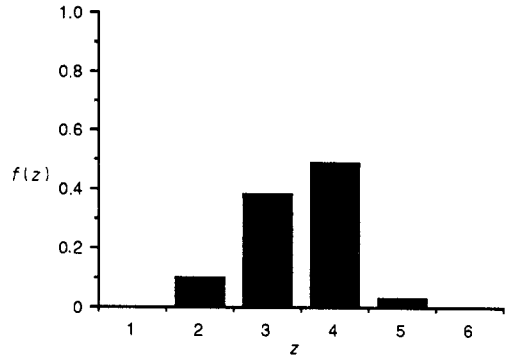

Figure 10. Distribution of coordination numbers ($C_0 = 0.5 - p/R = 0.5$).

Table 1. Different results on 'grain-by-grain' packings.

Reference	Packing mode	C	z
Bideau and Troadec (1984)	Analogue under gravity	0.84 ± 0.01	3.75 ± 0.1
Dodds (1975)	Analogue under gravity	—	4.72
Quickenden and Tan (1974)	Analogue under central force	0.830 ± 0.015	4
Visscher and Bolsterli (1972)	Numeric under gravity	0.82	—
Dodds and Kuno (1975)	Numeric under gravity	—	4.02
Bideau *et al* (1986)	Numeric under central force	0.83	4.1
Kausch *et al* (1971)	Numeric under central force	0.827 ± 0.004	—
Rubinstein and Nelson (1982)	Numeric under central force	0.825 ± 0.02	—
This work	Numeric under central force	0.835 ± 0.005	4.21 ± 0.05

0.84 (see table 1). Values greater than 0.82 are generally attributed to the presence of crystallised regions (Visscher and Bolsterli 1972, Bideau *et al* 1986, Quickenden and Tan 1974, Kausch *et al* 1971, Rubinstein and Nelson 1982). So it seems that the random 'grain-by-grain' packing is the 2D random packing with the maximum packing fraction and there is no distinction between the random 'grain-by-grain' packing and the random close packing in two dimensions. Nevertheless, there are some indications that a 2D close random packing really exists, the packing fraction being 0.87 ± 0.004 (Schreiner and Kratky 1982).

These results are in excellent agreement with our results from computer experiments obtained for low C_0-values and $p/\rho > 1$. Because they all use a 'grain-by-grain' building mode, simulated packings give similar values of C and z. In the analogic simulation of

Bideau and Troadec (1984), the bed was submitted to a vibration and crystallised regions were observed. Quickenden and Tan (1974) compressed a series of disks lying on a plane, each disk separated from the other by a large distance. Their experiments gave results very close to the preceding ones (see table 1). The theoretical mean coordination number in a 2D 'grain-by-grain' packing is 4 as each disk must bring two contacts into equilibrium and thus four bonds are created. In fact, crystallisation leads to a slightly higher value in numerical packings (table 1). Our results, obtained for low values of C_0 and $p/\rho > 1$ are in agreement with other simulation results. It is interesting to note that our packings exhibit some kind of order ($z > 4$) although no disk presents a coordination number of 6 (figure 9). The analogic measurements made by Dodds (1975) and Bideau and Troadec (1984) are mean values of coordination numbers evaluated on binary disk packings. The difference between the two results could be explained by the difficulty in differentiating an actual contact from a close neighbourhood in real packings.

So our program is able to simulate 'grain-by-grain' packings, but its major advantage is to simulate collective packings. The development of the characteristics of the packing built collectively ($p/R \leqslant 0.5$) with the initial density exhibits a limiting state in which arching effects are important. This limiting state can be found at $C_0 = 0.5$ and the following macroscopic minimum values are obtained: $C = 0.756 \pm 0.03$ and $z = 3.40 \pm 0.03$. As for the minimum packing fraction, no similar result has been published so far that we know of. Bideau *et al* (1986) have determined the minimum coordination number in a packing of disks which are stable under gravity. They made a digital simulation on a hexagonal network oriented in such a way that gravity would not be parallel to one of the network axes. Then they removed the bondings which were not necessary to the equilibrium of a particle or of the packing at random. The minimum found in this case was $z = 3.45 \pm 0.05$. Uhler and Schilling (1985) have calculated a lower value of $z = 3.416$ with a different stability criterion. These values are close to ours.

When C_0 varies for 2D packings built collectively (simulated with $p/R \leqslant 0.5$), a transition between two states is observed with a sharp variation in packing fraction and coordination number at an initial density of about 0.1.

If one assumes that this result can be extrapolated to 3D space, the critical initial density $(C_0)_3$ in three dimensions can be roughly estimated as follows. Let us suppose that for a 2D packing of disks the N disks are located according to a square network. If λ is the distance separating the edge of one disk from that of the next disk, then we get the relation $\pi R^2 = C_0(\lambda + 2R)^2$. Under these conditions the critical parameter λ for the transition is equal to $3.6R$ for $C_0 = 0.1$. From this we conclude that a disk assembly starts to have a collective behaviour when λ/R is about 3 or 4. Supposing now that this critical parameter λ/R remains unchanged in 3D, inversely it is easy to calculate the critical initial density $(C_0)_3$ for an assembly of spheres belonging to a cubic structure with a cell parameter $a = \lambda + 2R$. As $\frac{4}{3}\pi R^3 = (C_0)_3(\lambda + 2R)^3$, $(C_0)_3$ can be deduced from the relation

$$C_{0_3} = (4/3\sqrt{\pi})C_0^{3/2}.$$

If we put $C_0 = 0.1$, then we obtain $(C_0)_3 = 0.024$. Such a value is very often exceeded in elementary operations in chemical engineering such as the mixing of solids and the pouring or fluidising of particles, so that arching effects are likely to be expected.

5. Conclusion

Our algorithm allows us to simulate a collective packing of equal disks submitted to a central force. When using large moving steps, the classical case of packings built grain

by grain is found again. With a moving step of less than half the radius of the disks, the collective behaviour of the particles can be described; if the initial density increases, the packing fraction and mean coordination number drop to 0.76 and 3.4; those values are characteristic of a collective packing with arching effects only. Such results are qualitatively consistent with those in the experiments of Macrae and Gray (1961): they studied the packing fraction of a packing of spheres obtained after pouring them into a vessel. They noticed that this packing fraction reduced as the density of the falling spheres increased.

Appendix. Calculation of the area of a disk intersected by a circular ring

Let us consider a circular ring with centre C limited by two circles $\mathbb{C}_1$ and $\mathbb{C}_2$ of respective radii R_1 and R_2, and a disk $\mathbb{D}$ with centre P and radius R, at a distance d to centre C (figure A1). Let us denote by A_i $(i = 1, 2)$ the area of intersection of the disk $\mathbb{D}$ with the disk $\mathbb{C}_i$, and A_s the area of intersection of the disk $\mathbb{D}$ with the ring. Figure A1 shows that three cases must be considered for the calculation of A_s. Case 1 is

$$R_2 - R \leqslant d \leqslant R_1 - R$$

$$A_s = \pi R^2 - A_2.$$

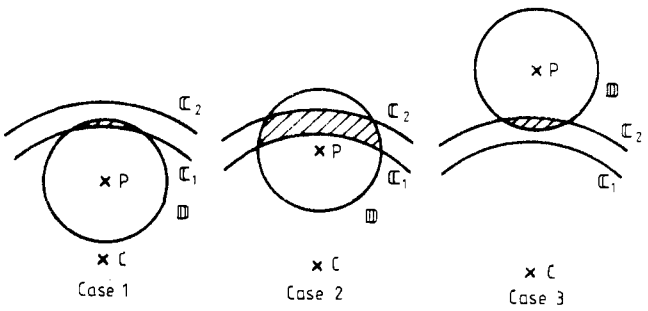

Figure A1. Intersection of a disk $\mathbb{D}$ with a circular ring.

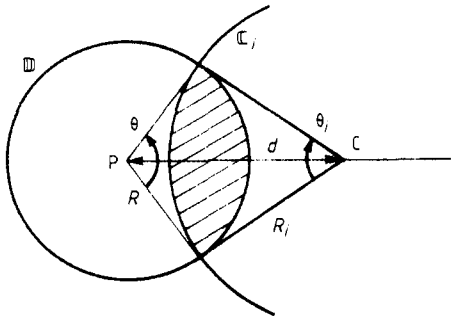

Figure A2. Area of intersection of a disk $\mathbb{D}$ with a disk $\mathbb{C}_i$.

Case 2 is

$$R_1 - R \leqslant d \leqslant R_2 + R$$

$$A_s = A_1 - A_2.$$

Case 3 is

$$R_2 + R \leqslant d \leqslant R_1 + R$$

$$A_s = A_1.$$

Then the problem becomes the evaluation of the area A_i of intersection of two disks (figure A2). This has been done using geometrical considerations:

$$A_i = (R^2/2)(\theta - \sin\theta) + (R_i^2/2)(\theta_i - \sin\theta_i)$$

with

$$\cos\theta = \{d^2 + [(R_i^2 - R^2)/d]^2 - 2R_i^2\}/2R^2$$

and

$$\cos\theta_i = \tfrac{1}{2}(d/R_i - R^2/dR_i + R_i/d)^2 - 1.$$

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