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RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

SOME GEOMETRICAL PROPERTIES OF PACKINGS OF EQUAL SPHERES IN CYLINDRICAL VESSELS.
PART III - BASIC MODEL AWAY FROM THE INFLUENCE OF WALL EFFECTS

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N.W. RIDGWAY
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ABSTRACT

An experimental study of the structure of random packings of equal spheres in cylindrical vessels, which indicated the existence of a continuous range, has been followed by an analytical investigation.

A model was developed on the basis that random packings, away from the influence of wall effects, can form by a process of expansion from the densest possible packing. Equations are derived connecting the mean void fraction, the mean number of points of contact, and other related properties. Both the three-dimensional and the two-dimensional cases are considered, and are found to have similar features.

The equations give values which are in good agreement with available experimental results and with values computed by other means.

PREFACE

This report is part of a series on "Some Geometrical Properties of Packings of Equal Spheres" as follows:

Part I Exploratory Study of Random Packings in Small Cylindrical Vessels.
G. A. Tingate, A.A.E.C. report in preparation.

Part II The Cylindrically Ordered Packing.
F. A. Rocke, A.A.E.C. report in preparation.

Part III Basic Model away from the Influence of Wall Effects.
N. W. Ridgway, G.A. Tingate, AAEC/E202.

Part IV Extension of Model to Outer Region of Semi-infinite Vessel with Plane Wall.
G. A. Tingate, A.A.E.C. report in preparation.

Part V Adaptation of Model to Packings in Cylindrical Vessels.
G. A. Tingate, A.A.E.C. report in preparation.

Part VI Discussion and Conclusions.
N. W. Ridgway, F. A. Rocke and G. A. Tingate, A.A.E.C. report in preparation.

CONTENTS

1. INTRODUCTION

In 1966 the Australian Atomic Energy Commission completed a feasibility study of a high temperature gas-cooled reactor system based on the pebble bed concept, using spheres of fuelled beryllium oxide. The work reported here stems from a study of some of the properties of random packings of equal spheres in transparent cylindrical vessels with vertical axes. A knowledge of the structure of such packings is relevant to such areas as fuel loading and reactivity, flow of spheres, coolant flow, heat transfer and thermal stresses in the sphere material.

Packings were prepared by a variety of methods over a substantial range of cylinder-to-sphere diameter ratios, and the results indicated that a continuous range of random packings is possible (Tingate 1969). The limits of the range are not known with certainty, but the overall void fractions of all the packings were within the range 0.36 and 0.42. Smith et al. (1929) and Bernal and Mason (1960) reported observed ranges of 0.36 to 0.45 and 0.36 to 0.40 respectively.

When the number of spheres touching the cylindrical wall was plotted against the total number of spheres in the packing, most of the points were found to lie reasonably close to a line of best fit. A few points were well away from this line, but the packing methods in these cases were such as might be expected to result in radial bias. Methods involving non-uniform impact on the top surface of the packing fall into this category. No attempt had been made to produce radial bias in any of the packings which were close to the line of best fit.

It was also apparent from the experimental results that the mean void fraction of the wall region did not bear a unique relationship to that of the central region. Furthermore the wall region was much more sensitive to the packing method than the central region.

It was therefore considered desirable to determine the properties of radially unbiased packings, and the range over which they can form, to provide a foundation for the investigations. This information might further indicate the means by which an unbiased packing could be prepared at will at or near any desired point in the range. The resulting structure would be unique, so a check could be made as to whether the desired packing had in fact been obtained merely by knowing the diameter and height of the packing and the number of spheres contained. Where a packing is known to be biased, additional determinations have to be made in the wall region, but this may not be readily practicable in some applications.

2. ANALYSIS

2.1 General

Owing to the difficulty of computing the properties of packings in finite cylinders, attention was directed to the infinite case. The approach adopted was to regard any unbiased packing in a semi-infinite vessel with a plane wall as having been formed by some process of expansion from the densest possible packing, the rhombohedral array. The initial studies, reported here, were confined to the infinite three-dimensional model away from the influence of wall effects, and its two-dimensional counterpart. The extension of the model to the wall region of the three-dimensional case, and its final adaptation to the finite cylindrical case, are the subjects of Parts IV and V of this series.

2.2 Three-dimensional Case away from Wall Effects

An equation was derived, relating the mean void fraction ϵ to the mean number of points of contact n between each sphere and its neighbours, as follows:

$$1 - \epsilon = \frac{\pi}{\sqrt{3(12 - \frac{n}{2})}} \quad . \tag{1}$$

This equation can be derived by considering some of the properties of packings of spheres of unit diameter. These properties are expressed in terms of the effective radial distance ρ of the centres of neighbouring spheres from the centre of a reference sphere. The relationship between ρ and the mean volume V associated with a sphere is:

$$V = a\rho^3 \quad , \tag{2}$$

where a is a constant.

The mean void fraction ϵ is, by definition, given by

$$\epsilon = 1 - \frac{V_s}{V} \quad , \tag{3}$$

where V_s is the volume of a sphere,

or
$$\epsilon = 1 - \frac{V_s}{a\rho^3} \quad . \tag{4}$$

At this stage a simple physical relationship between n and ρ could not be postulated, so it was taken to be of the form:

$$n = b - c\rho^\gamma \, , \tag{5}$$

where b, c and γ are assumed to be constants, that is, n decreases with increasing void fraction, which itself increases with increasing ρ. There was no certainty at this point that γ would be an integer, but it was thought that it might correspond to some simple geometric property of the system, for example, a linear dimension ($\gamma = 1$), a surface ($\gamma = 2$) or a volume ($\gamma = 3$).

From (5),

$$\rho = \left(\frac{b - n}{c}\right)^{\frac{1}{\gamma}} \quad , \tag{6}$$

and from (2) and (6)

$$V = a\left(\frac{b - n}{c}\right)^{\frac{3}{\gamma}} \quad . \tag{7}$$

Hence the mean void fraction is given by:

$$1 - \epsilon = \frac{V_s}{a} \cdot \left(\frac{b - n}{c}\right)^{-\frac{3}{\gamma}} . \tag{8}$$

If two pairs of values, ϵ_0, n_0 and ϵ_1, n_1 are known, a, b and c can be eliminated to give

$$1 - \epsilon = \left[(1 - \epsilon_0)^{-\frac{\gamma}{3}} \cdot \frac{n - n_1}{n_0 - n_1} - (1 - \epsilon_1)^{-\frac{\gamma}{3}} \cdot \frac{n - n_0}{n_0 - n_1}\right]^{-\frac{3}{\gamma}} . \tag{9}$$

The values at the assumed starting point, the rhombohedral array, are

$$\epsilon_0 = 1 - \frac{\pi}{3\sqrt{2}} = 0.2595 \text{ when } n_0 = 12 \, .$$

The only values available for random packings are as follows:

ϵ	Bernal and Mason (1960)			Smith et al. (1929)
	Points of Contact (n)	Near Contacts	Total	Contacts *
0.38	6.4	2.1	8.5	9.0
0.40	5.5	1.6	7.1	8.6

* Smith et al. presented results for five random packings in all, but no distinction was made between points of contact and near contacts. Both Smith et al. and Graton and Fraser (1935) discussed the possibility that random packings may consist of mixed clusters of the rhombohedral and cubic arrays. Smith et al. derived an equation connecting mean void fraction and mean number of contacts on this basis, which agreed well with their experimental results, but not with the results of Bernal and Mason. Wadsworth (1960) also expressed doubts about the results of Smith et al. and proposed a correction which brings them more into line with the results of Bernal and Mason.

The only values of interest to this study are those in the first two columns. Either pair of values could have been used to give ϵ_1 and n_1 in Equation 9 but the second (with $n = 5.5$) was selected to give the widest possible range. This gives a general equation for ϵ and n with only γ unknown.

The portion of the curve between $n = 12$ and $n = 6$ is found to be virtually unaffected by putting $\gamma = 1$, 2 or 3. When the curves are extended back to $n = 0$ they diverge, but even there the differences are small, the corresponding values of ϵ being 0.4924, 0.4875 and 0.4830.

The observed and computed void fractions for Bernal and Mason's other point ($n = 6.4$) agreed with 0.7 per cent ($\gamma = 1$), 0.9 per cent ($\gamma = 2$) and 1.0 per cent ($\gamma = 3$).

The only other relevant experimental results in the literature are those of Denton (1953) who found that the mean void fraction of packings after recirculation of ¼ in. marbles in a 10 in. diameter cylindrical vessel was independent of the void fraction before recirculation commenced, as shown in the following table:

Expt. No.	Shape of Base	Overall Void Fraction	
		Initial value	Final steady value
1	Hemisphere	0.3917	0.3955
2	"	0.3931	0.3950
3	"	0.3924	0.3947
4	"	0.3919	0.3945
5	"	0.3911	0.3955
6	Cone	0.3936	0.3958
7	"	0.3747	0.3950
8	"	0.3950	0.3954
9	"	0.3860	0.3954
10	"	0.3893	0.3950

The mean number of points of contact is not known, but as discussed by Bernal and Mason the most probable average would seem to be six, as each sphere may be considered in general to rest on three others and in turn to support another three.

In a computer programme to generate random packings of spheres in finite cylinders (Clancy 1966), the computational scheme was to place each sphere in turn at the lowest equilibrium position on top of the packing without disturbing the other spheres. The computed values were found to be $\epsilon = 0.397$ and $n = 6.10$.

Returning to the three calculated values of ϵ at $n = 0$, it can be seen that they are successively closer to the void fraction of the loosest regular packing, the cubic array, for which

$$\epsilon = 1 - \frac{\pi}{6} = 0.4764 \quad .$$

Replacement of Bernal and Mason's experimental values by $\epsilon_1 = 0.4764$ and $n_1 = 0$ gives rather low values of ϵ when $n = 6$ (0.3804, 0.3835 and 0.3866 for $\gamma = 1$, 2 and 3). However, when the value $\gamma = 6$ is used, Equation 9 converts directly into Equation 1, which on evaluation for various n gives:

for $n = 0, \ \epsilon = 1 - \dfrac{\pi}{3\sqrt{4}} = 0.4764$ (same ϵ as cubic array),

for $n = 6, \ \epsilon = 1 - \dfrac{\pi}{3\sqrt{3}} = 0.3954$ (same ϵ as orthorhombic array),

and for $n = 12, \ \epsilon = 1 - \dfrac{\pi}{3\sqrt{2}} = 0.2595$ (rhombohedral array) .

The observed and computed void fractions for Bernal and Mason's two points agree within 0.9 per cent ($n = 5.5$) and 2.3 per cent ($n = 6.4$).

Equation 1 and various points of interest, including the four regular arrays and the computed point, are plotted in Figure 1. Observed and calculated values of ϵ and n are given in Table 1.

The value $\gamma = 6$ was next used to determine the values of a, b and c in Equations 2 and 5. We have:

$n = 0$ when $V = 1$ (same V as cubic array),

$n = 6$ when $V = \dfrac{\sqrt{3}}{2}$ (same V as orthorhombic array),

$n = 12$ when $V = \dfrac{1}{\sqrt{2}}$ (rhombohedral array).

Further, $\rho = 1$ in the rhombohedral case, giving

$$a = \frac{1}{\sqrt{2}} , \quad b = 24 \text{ and } c = 12.$$

Hence Equations 2 and 5 become

$$V = \frac{1}{\sqrt{2}} \rho^3 , \qquad (10)$$

and

$$n = 12 \, (2 - \rho^6) , \qquad (11)$$

from which it follows that

$$n = 24\,(1 - V^2)\ . \tag{12}$$

It should be noted that the best fit of Bernal and Mason's experimental points is obtained by putting $\gamma = 4$. The computed void fractions then differ from the observed ones by –0.5 per cent ($n = 5.5$) and + 0.7 per cent ($n = 6.4$). Further analytical and experimental work to establish the correct relationship beyond reasonable doubt included a study of the two-dimensional case as follows:

2.3 Two-dimensional Case away from Edge Effects

This study was concerned with the structure of discs of unit diameter, away from edge effects, in a vessel consisting of two parallel faces whose distance apart equals the disc thickness. It was more convenient to use equal spheres for experimental work, and to calculate void fractions in terms of the equivalent discs. The two-dimensional case might be expected to cast some light on the wall region of a three-dimensional packing, but the latter is complicated by the fact that spheres intruding from the central region can hold apart some of the spheres touching the wall. It should also be noted that the condition for static equilibrium gives four points of contact in the two-dimensional case compared with six in the three-dimensional case. These are two-thirds and half respectively of the maximum possible number of points.

An equation:

$$1 - \epsilon = \frac{\pi}{2\sqrt{5 - \frac{n}{3}}}\ , \tag{13}$$

similar to Equation 1 was derived by proceeding on the same basis as for the three-dimensional case.

We have

$$A = a'\rho^2 \tag{14}$$

$$\epsilon = 1 - \frac{A_d}{A}\ , \tag{15}$$

and A_d is the area of a disc and A is the mean area associated with each disc,

or

$$\epsilon = 1 - \frac{A_d}{a'\rho^2}\ . \tag{16}$$

Further

$$n = b' - c'\rho^\gamma\ , \tag{17}$$

leading to the relationship

$$1 - \epsilon = \left[(1-\epsilon_0)^{-\frac{\gamma}{2}} \cdot \frac{n - n_1}{n_0 - n_1} - (1-\epsilon_1)^{-\frac{\gamma}{2}} \cdot \frac{n - n_0}{n_0 - n_1}\right]^{-\frac{2}{\gamma}}\ , \tag{18}$$

which can be evaluated for any γ if ϵ_0, n_0 and ϵ_1, n_1 are known.

Experimental values for random two-dimensional packings could not be found in the available literature. A two-dimensional vessel was therefore prepared with two parallel transparent plane walls 1 in. apart, for use with 0.990 in. diameter aluminium spheres (see Figure 2). The edges of the vessel were lined with wooden strips cut to give an irregular curved profile. The test area, a 32 in. x 28 in. rectangle, was marked with a 4 in. x 4 in. grid to facilitate the recording of observations. The mean void fraction and the mean number of sphere to sphere contact points were determined for the widest possible range of random packings, and the results are given in Figure 3.

The computer programme (Clancy 1966) was modified and used to apply the same computational scheme to the two-dimensional case with the following results:

Property	Computed Value	
	Three-dimensional case	Two-dimensional case
Mean number of points of contact (n)	6.10	4.00
Mean void fraction (ϵ)	0.397	0.185
Mean occupancy fraction ($1 - \epsilon$)	0.603	0.815

Several possible two-dimensional models were next considered. All had the densest possible packing as the starting point, where n = 6 and each disc or sphere is associated with a unit wall area equal to the area of the circumscribed hexagon. At the other terminal point, where n = 0, the circumscribed square and the circumscribed triangle were considered. The corresponding curves are plotted in Figure 3, but it can be seen that the computed and experimental points fall well away from both.

Now we have:

$$\epsilon = 1 - \frac{\pi}{2\sqrt{3}} \quad \text{when } n = 6,$$

which suggests an equation of the form:

$$\epsilon = 1 - \frac{\pi}{2\sqrt{Pn+Q}} \quad , \text{ where P and Q are constants.}$$

Hence $6P + Q = 3$,

while from Clancy's computed point,

$$4P + Q = 3.715$$

giving $\quad P = -0.358 \quad \text{and} \quad Q = 5.145.$

Using these values, ϵ is calculated to be

$$1 - \frac{\pi}{2\sqrt{4.071}} \quad \text{when } n = 3.$$

This suggests $1 - \frac{\pi}{2\sqrt{4}}$, and when P and Q are recalculated on this basis, Equation 13 is obtained.

From this equation,

when $\quad n = 0, \ \epsilon = 1 - \frac{\pi}{2\sqrt{5}} = 0.2975$ (significance unknown),

when $\quad n = 3, \ \epsilon = 1 - \frac{\pi}{2\sqrt{4}} = 0.2146$ (same ϵ as circumscribed square),

when $\quad n = 6, \ \epsilon = 1 - \frac{\pi}{2\sqrt{3}} = 0.0931$ (circumscribed hexagon).

Equation 13 can be derived directly from Equation 18 by using any two of these points and putting $\gamma = 4$. This curve is also plotted in Figure 3, together with points representing three regular two-dimensional arrays*. It gives a mean occupancy fraction of 0.8203 when n = 4, compared with Clancy's figure of 0.815.

It would be difficult to resolve these differences further by experiment since regular areas form very readily in two-dimensional packings and prevent one from being certain that random packings have in fact been obtained. The vessel was tilted almost to the horizontal to prepare the looser packings but it was not possible to obtain values of n significantly less than 3.

The value $\gamma = 4$ was next used to determine the values a', b' and c' in Equations 14 and 17, giving

$$A = \frac{\sqrt{3}}{2}\,\rho^2 , \tag{19}$$

and

$$n = 3\,(5 - 3\,\rho^4) , \tag{20}$$

from which it follows that

$$n = 3\,(5 - 4\,A^2) . \tag{21}$$

3. DISCUSSION

The similarity of the two-dimensional and three-dimensional equations, and the similar dispositions of some of the experimental and regular packing points in Figures 1 and 3, do not in themselves demonstrate the validity of the model. Further experimental evidence is desirable, the values of ϵ and n for three-dimensional packings of equal spheres after recirculation being of particular interest. Even with this packing the number of points of contact could be slightly less than 6, say, when a sphere is supported at two points on its lower hemisphere and constrained by a third point at or just above its equator.

It is nevertheless appropriate to consider some possible implications of Equation 1. It throws some light on the range of random packings and the factors governing the densest and loosest practical packings.

As stated above, the 'normal' random packing is considered to have 6 points of contact per sphere and a mean void fraction of 0.3954. It is envisaged as a stable structure when at rest, yet having mobility throughout when gravitational flow is initiated from the bottom. If such a packing is densified, say by vibration, the spheres make further contacts with their neighbours. Some are now supported by four other spheres, and if one such supporting sphere is displaced downwards the supported sphere does not necessarily move. As the packing is densified further, the point is reached where every sphere in the packing is supported by four others and forms a support for four others. At this point the packing may be regarded as a redundant structure, largely if not completely devoid of mobility. Denton reported a void fraction of 0.368 after prolonged jolting, and stated that it seemed improbable that a value of less than 0.36 could be attained. Equation 1 gives $\epsilon = 0.3587$ when n = 8; this might therefore be the densest possible random packing, in the absence of plane or cylindrical boundaries, which strongly encourage the formation of even denser, regular, arrays.

The limit at the loose end of the range is not so straightforward. If it lies on the curve in Figure 1, it must clearly fall well short of the point where n = 0. However it will not necessarily lie on the curve. The criterion for stability is that there must be three points of support for each sphere, and if this were in fact met, the loose packings would lie on the vertical line joining the 'normal' random packing and the cubic array.

The study has been extended to the wall region of three-dimensional packings, on the basis of Equation 1, and further supporting evidence of its validity has been found. This will be reported in Part IV.

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* The two broken curves have been obtained by putting $\gamma = 4$ in Equation 18 and using the values in the figure.

4. NOTATION

ρ = Mean radial distance of the centres of neighbouring spheres (or discs) of unit diameter about the centre of a reference sphere (or disc).

V_s = Volume of sphere of unit diameter.

V = Volume of region associated with each sphere in a three-dimensional packing.

A_d = Area of disc of unit diameter.

A = Area of region associated with each disc in a two-dimensional packing.

n = Mean number of points of contact of a sphere (or disc) with its neighbours.

ϵ = Mean void fraction of region.

5. ACKNOWLEDGEMENT

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TABLE 1

OBSERVED AND CALCULATED MEAN VOID FRACTIONS FOR THREE-DIMENSIONAL PACKINGS OF EQUAL SPHERES

Mean Number of Points of Contact (n)	Mean Void Fraction (ϵ)						
	Observed	Calculated from Equation 9					
		$\gamma = 1$	$\gamma = 2$	$\gamma = 3$	$\gamma = 4$	$\gamma = 5$	$\gamma = 6$*
12.0	0.2595	0.2595	0.2595	0.2595	0.2595	0.2595	0.2595
11.0		0.2817	0.2829	0.2842	0.2856	0.2870	0.2886
10.0		0.3031	0.3051	0.3073	0.3096	0.3120	0.3144
9.0		0.3236	0.3262	0.3290	0.3318	0.3347	0.3377
8.0		0.3433	0.3463	0.3493	0.3524	0.3556	0.3587
7.0		0.3622	0.3654	0.3685	0.3716	0.3748	0.3779
6.4	0.38	0.3732	0.3764	0.3795	0.3825	0.3856	0.3887
6.0	0.39–0.395	0.3804	0.3835	0.3866	0.3896	0.3925	0.3954
5.5	0.40	0.3893	0.3922	0.3952	0.3981	0.4009	0.4036
5.0		0.3980	0.4008	0.4036	0.4063	0.4090	0.4115
4.0		0.4148	0.4173	0.4197	0.4221	0.4243	0.4264
3.0		0.4311	0.4331	0.4350	0.4369	0.4386	0.4402
2.0		0.4468	0.4482	0.4495	0.4508	0.4520	0.4531
1.0		0.4619	0.4626	0.4633	0.4640	0.4646	0.4651
0.0		0.4764	0.4764	0.4764	0.4764	0.4764	0.4764

* Same as Equation 1

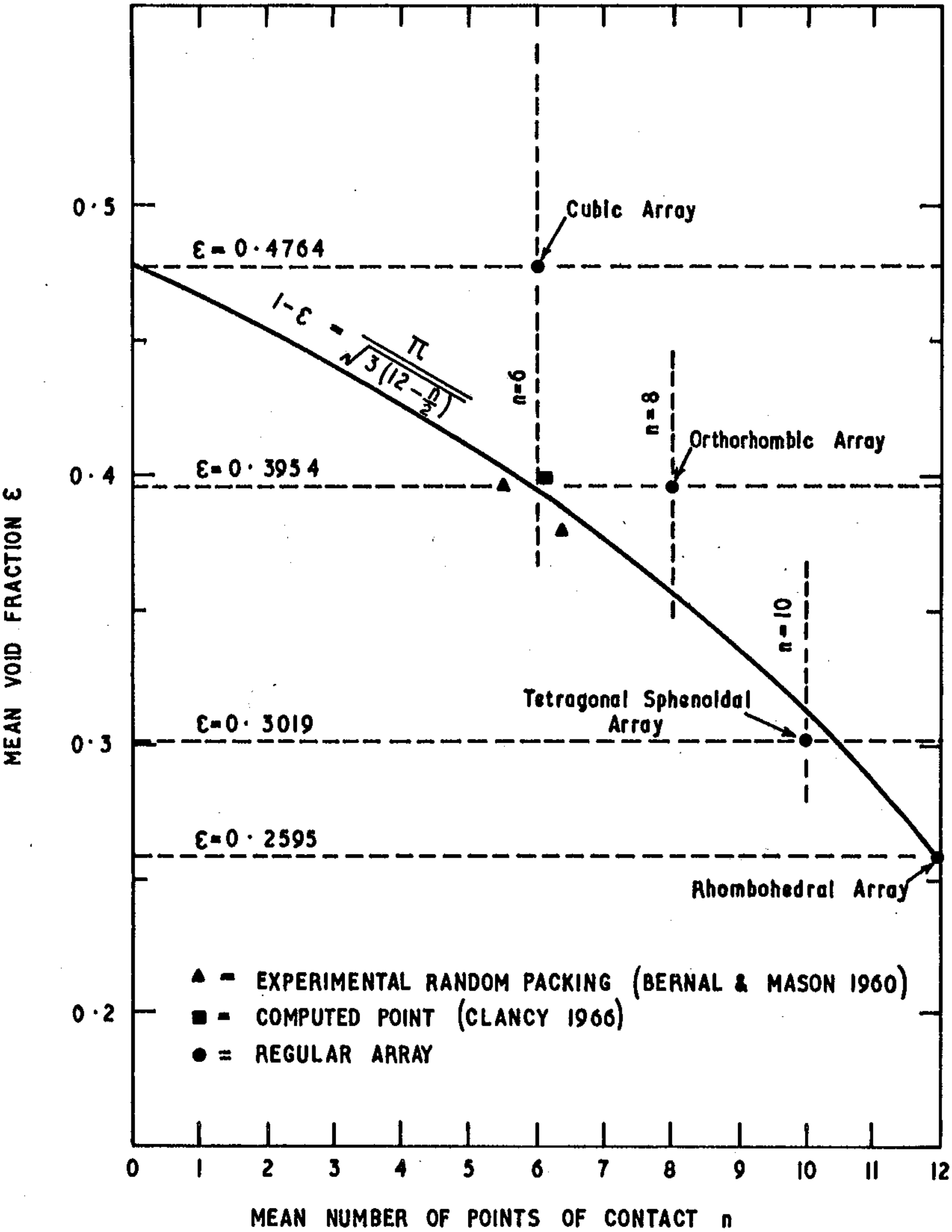

FIGURE 1. PROPERTIES OF THREE-DIMENSIONAL PACKINGS AWAY FROM WALL EFFECTS

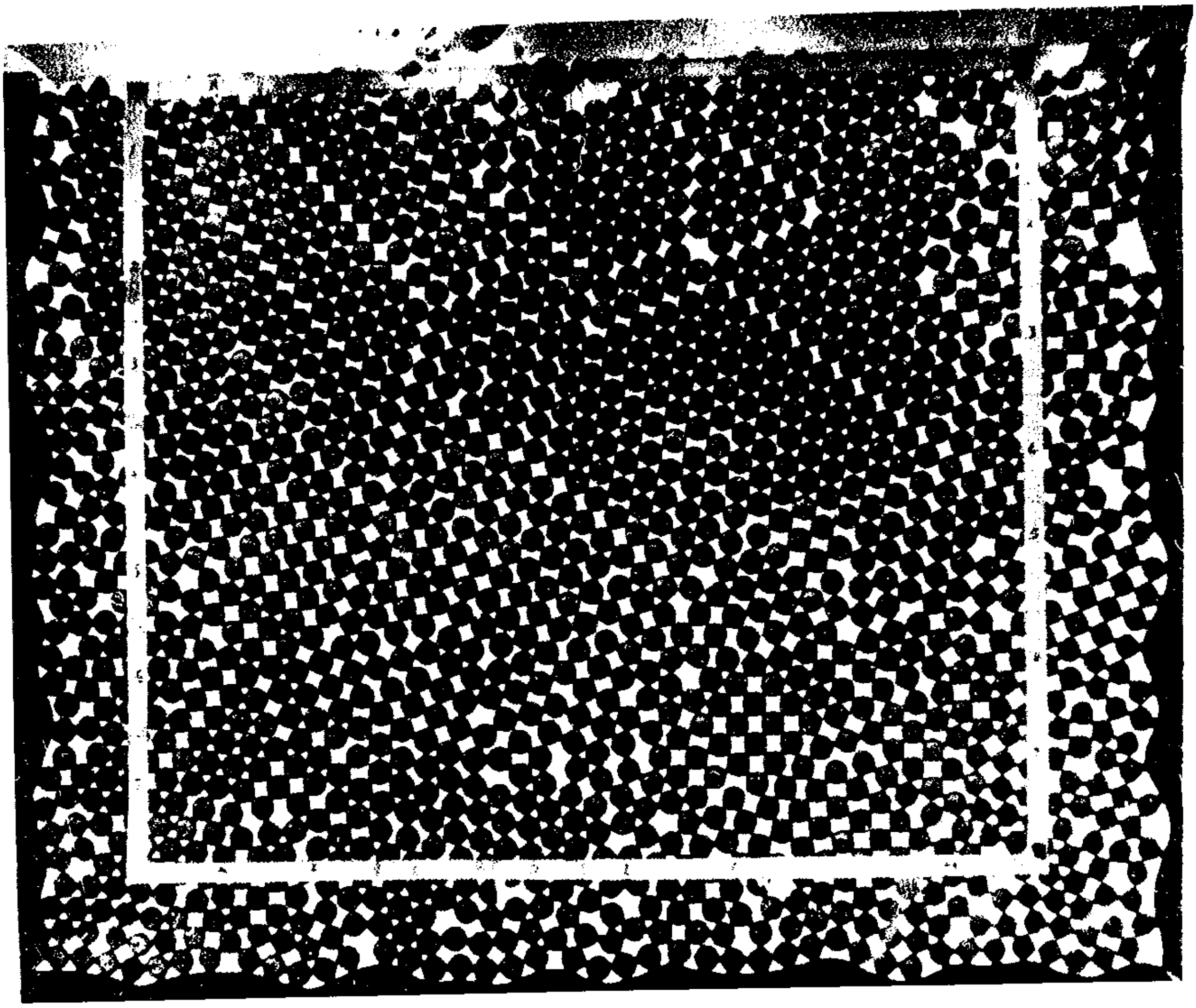

FIGURE 2. TYPICAL TWO-DIMENSIONAL PACKING
(1 in. spheres, 32 in. × 28 in. test area)

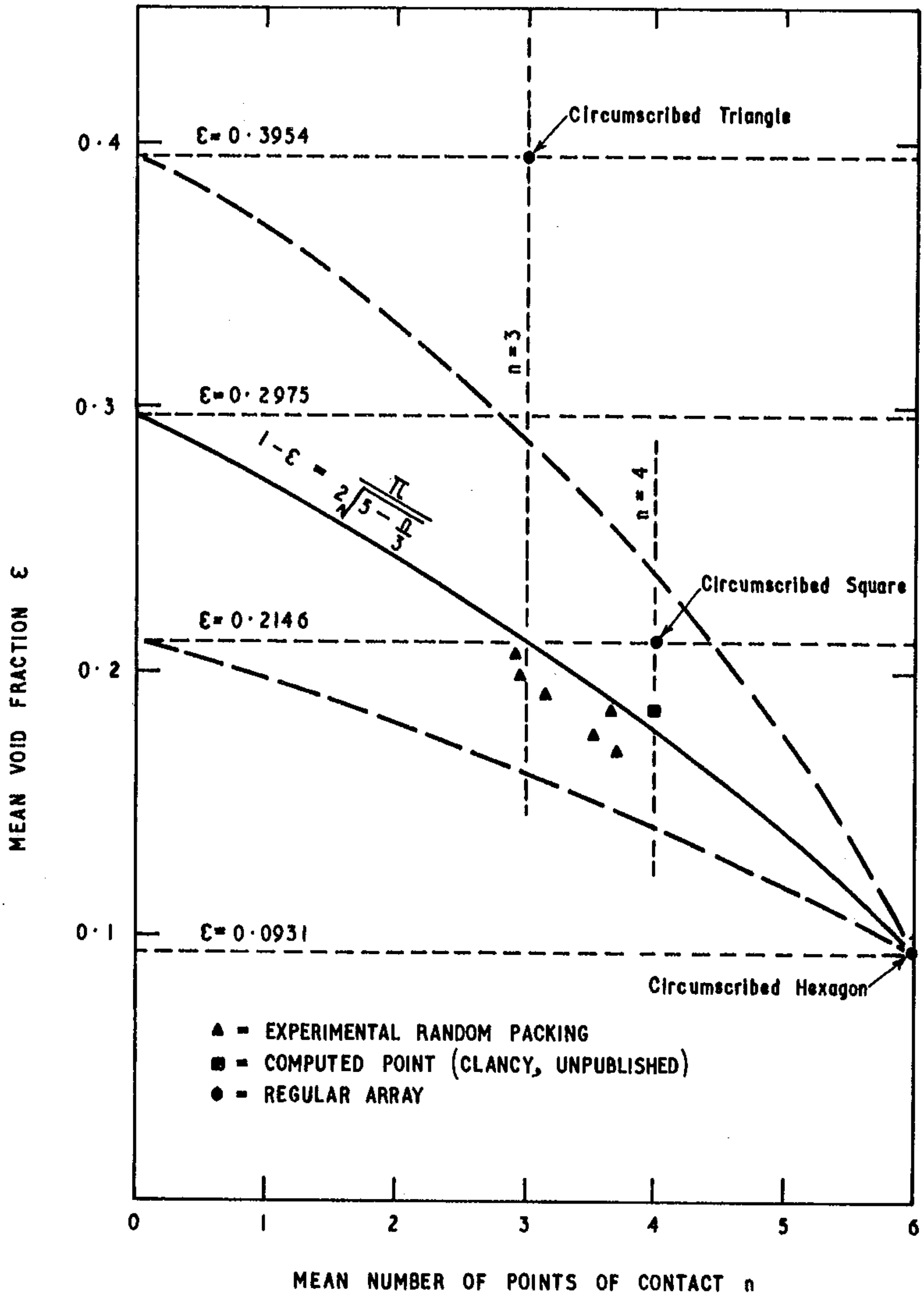

FIGURE 3. PROPERTIES OF TWO-DIMENSIONAL PACKINGS AWAY FROM EDGE EFFECTS