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REPRESENTATION OF PACKING IN A CLASTIC SEDIMENT

Northampton College, London, England

I. J. SMALLEY

ABSTRACT. A radial distribution function is a more accurate representation of the packing structure of clastic sediments than the regular unit cell. Existing methods of determining distribution functions can be modified to make them more suitable for use on random packs of irregular particles as represented by typical clastic sediments.

TABLE OF SYMBOLS

d — diameter of particles
r — distance from reference particle
ρ_0 — mean aggregate density
$\rho(r)$ — density function
W(r) — probability function
N — number of particles
N_{av} — average number of particles at distance r
V — volume of the system
n — number of interparticle distances measured
p, q — specific particles
x, y, z — coordinates to fix particle positions

INTRODUCTION

The packing of the particles in a clastic sediment has been compared to the regular packing of equal spheres, particularly by Graton and Fraser (1935) whose long, detailed paper is still quoted as a basic reference. It is generally recognized that this gives a very imperfect analogue for a clastic sediment since it ignores so many features of the actual aggregate. Much over-simplification and confusion can be caused by the concept of regularity applied to particle aggregates. Graton and Fraser stress the importance of six fundamental packings, which are in fact only four packings, and there is little justification in suggesting that these four arbitrarily chosen packings bear any relationship to the packing characteristics of the particles in a clastic sediment. However even modern works continue to use the regular sphere pack analogy in referring to the structure of particle aggregates.

Thus a model of a clastic sediment exists; it is represented as a regular structure of equal spheres and is admittedly imperfect. The problem is to improve it and yet give a model both comprehensible and useful. A number of modifications are needed to render the model nearer reality; the four most important in order of importance are (1) a random instead of a regular structure, (2) a range of particle size, (3) other shapes as well as spheres, and (4) orientation effects. In this paper the first modification will be considered.

Regular structures can be classified by three factors: density, coordination number, and symmetry. The structures considered by Graton and Fraser have a range of packing density from 0.51 to 0.74 and coordination numbers of 6, 8, 10, and 12. The coordination number indicates how many particles touch each particle in the structure. It has been shown that the coordination number of a close random pack of equal spheres is of the order of 8.5 (Marvin, 1937; Bernal and Mason, 1960), and investigations with packs of steel and nylon spheres (Scott, 1960; Rutgers, 1962) have confirmed that the pack density is about 0.6. This is of the order of density observed in actual particle sediments. The random pack has little symmetry and cannot be represented by a unit cell. A unit cell represents the neighbor relationships of each particle in a regular aggregate. The long-range order of a regular aggregate allows it to be represented by a relatively simple repeating unit. A random aggregate has only short-range order and cannot be represented by a simple repeating unit. The method of representation used for random packs shows the radial distribution of particles about a typical particle. The geometrical effects of the short-range order cause a variation in density around each particle. A measure of this variation is typical of an aggregate.

THE RADIAL DISTRIBUTION FUNCTION

Consider any particle p in a random pack of equal spherical particles; the number of particles in a spherical shell of thickness dr, at distance r from p (provided r is large), will be $4\pi r^2\,dr\,\rho_0$ (where ρ_0 = the average density N/V). If r is small, short-range order effects are felt, and a density function is required. A graph of this function $\rho_{(r)}$ against r (fig. 1) shows the density

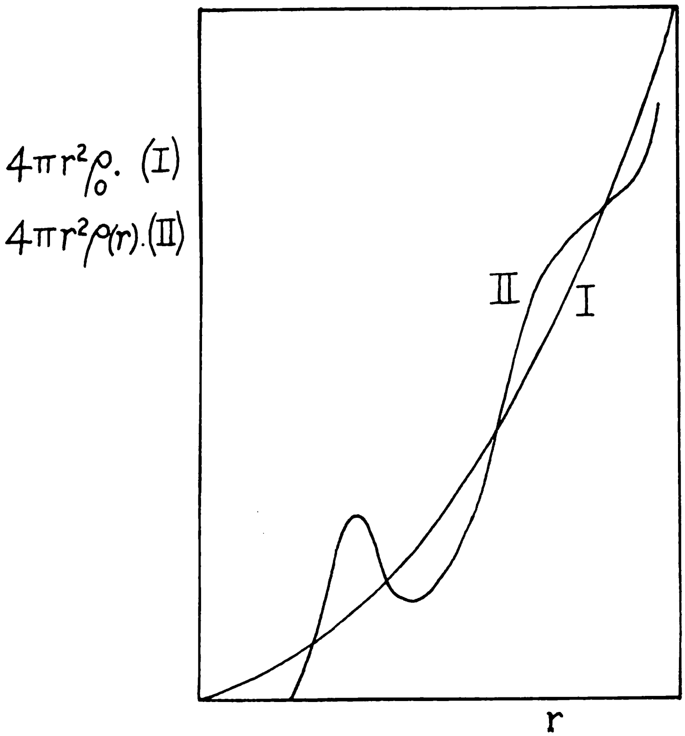

Fig. 1. Graph of $4\pi r^2\rho_0$ against r (I) and $4\pi r^2\rho_{(r)}$ against r (II); r is the distance from the reference particle, ρ_0 is the average aggregate density, and $\rho_{(r)}$ is the density function. These curves apply to a random aggregate of equal spheres.

variations round each particle in the aggregate. The diffuseness of the first peak is due to the approximate nature of the curve; no values of r less than d actually occur.

Related to the density function is a probability function W(r), which expresses the probability that the centers of two specified particles p and q should lie at distance r apart. This probability will be affected by the short-range order in the pack in the same way as the local density. If r is large, $W(r) = 1$, and since the particles cannot interpenetrate, when $r<d$, $W(r) = 0$. The density and probability functions have the same dependence on r. The probability that any particle q will lie at distance r from p is proportional to the average number of particles to be found at distance r from p. If the distribution is completely random then $\rho_{(r)} = \rho_0$ and $W(r) = 1$, thus $\rho_{(r)} = \rho_0 W(r)$. It will be seen that the points in figure 2 where $W = 1$ correspond to the points in figure 1 where curve II crosses curve I, i.e. where $\rho_{(r)}/\rho_0 = 1$. W depends only on the distance r between p and q in an aggregate of equal spheres. The aggregate is represented by the graph of W(r) against r. This graph can be determined experimentally. One technique can be illustrated by reference to the work of Morell and Hildebrand (1936). They determined the distribution

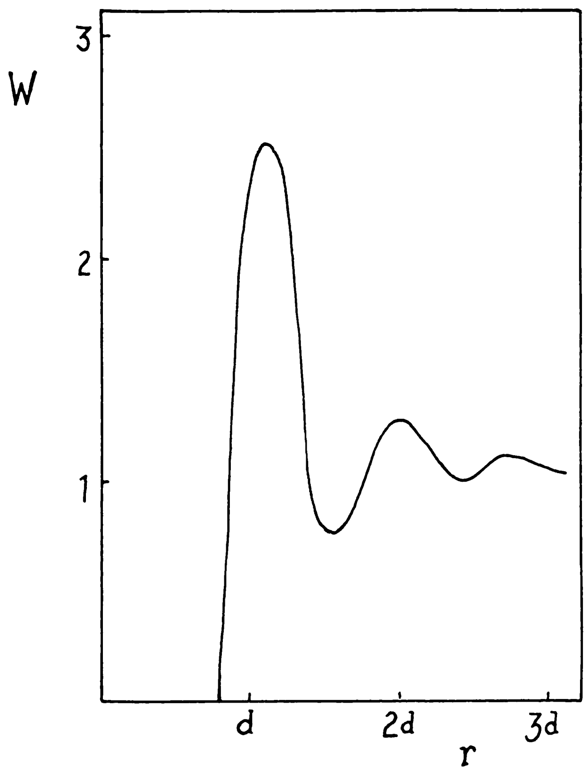

Fig. 2. Graph of W against r for a random aggregate of equal spheres. W is the probability function, r is the interparticle distance, and d is the sphere diameter.

function variation for random packs of equal spheres. For close random packs they used a pack of glass spheres. and for packs of lower density they used gelatine spheres partially supported by being immersed in a gelatine solution. Seven gelatine spheres were marked, and distances between these seven were measured. The positions of the marked spheres were observed. and coordinates (x, y, z) noted for each one. Values of Δx. Δy. and Δz were obtained by subtraction. For each pair the interparticle distance was given by

$$r = (\Delta x^2 + \Delta y^2 + \Delta z^2)^{1/2}$$

The distances between all possible pairs of marked spheres were calculated, and the number of times each distance occurred was tabulated. If this number be n then the total number of measurements obtained from the series can be designated $\sum_0^\infty n$ and $n/\sum_0^\infty n$ is the relative frequency with which this particular distance occurred in the series; or it is the relative chance that a particular sphere would at a certain time be found at a given distance r from a particular arbitrarily chosen reference sphere. Since there are N spheres the chance that any one of them would at that time be at distance r from the reference sphere is

$$(N-1)\, n/\sum_0^\infty n$$

or this is the probable number of spheres which at any one time would be found at a distance r from the reference one. The number which would probably be found within a spherical shell of inner radius r_1 and outer radius r_2 is

$$(N-1)\sum_{r_1}^{r_2} n/\sum_0^\infty n$$

and the number per unit volume within this shell would be

$$(N-1)\sum_{r_1}^{r_2} n/\sum_0^\infty n \int_{r_1}^{r_2} 4\pi r^2\, dr$$

Hence the ratio of the density at r to the overall density is

$$V(N-1)\sum_{r_1}^{r_2} n/N\sum_0^\infty n \int_{r_1}^{r_2} 4\pi r^2\, dr$$

and this represents W. On integration the expression becomes

$$W = 3V(N-1)\sum_{r_1}^{r_2} n/4\pi N\sum_0^\infty n\,(r_2^3 - r_1^3)$$

From this equation and measurements of sphere positions the value of W for each value of r can be calculated. The procedure in the above experiment is difficult and tedious, and it can hardly be recommended as a method of studying clastic sediments; a more flexible system is required. It can be supplied by the digital computer.

There are two general methods of simulating a random pack with the aid of a digital computer. Both are Monte Carlo methods; problems are solved by subjecting random numbers to numerical processes. A good introduction to this subject is that by Hammersley and Morton (1954). The two methods of simulating a particle aggregate depend on two completely different principles. One requires particles to be added to a random array until no more can be added: the other starts with a close packed array ($\rho_0 = 0.74$) of maximum density and by giving particles random displacements produces a random array of decreased density. Alder, Frankel, and Lewinson (1955) have applied the first method to an aggregate of spherical particles. A unit cube ($V = 1$) was set up, and the coordinates of a center of a sphere inside that cube were specified by a random nine digit number. The first three digits specified the x coordinate, the next three the y, etc. Additional particles were introduced into the unit cube at positions indicated by new random nine digit numbers. Particles were left in the box if they did not overlap any already there. To overcome inaccuracies due to surface effects of the small sample volume, special boundary conditions were applied. On all sides of the cube identical cubes were built. The computer calculated for each new particle the distance to each particle in the central box or to its reflection in an adjacent box, whichever was nearer. From these measurements the relative frequency of the various distances can be found and W calculated for values of r as in the Morell and Hildebrand method. The computers available to Alder, Frankel, and Lewinson were limited in capacity, and it was found that a particle density of about 0.2 could not be exceeded because of the frequency of occurrence of overlaps. This value is too low to have any relevance to the problem of the structure of clastic sediments, but the method has great possibilities. As computers are developed with larger stores and faster operation a realistic density will be obtainable, and it should be possible to program for a variation in particle size and perhaps shape.

These model methods were originally developed to study the structure of liquids. The liquids were considered as random aggregates of molecular particles. Their one great disadvantage for this application was the lack of any way of simulating chemical forces between the molecules. This disadvantage does not apply in the case of clastic sediments.

Reliance on the computer to set up a more or less exact model means complication and expense. Monte Carlo methods can be used on a limited scale to produce a reasonable analogue of a particle pack from which useful information may be gleaned. Prins (1931) has shown that a distribution function derived in two dimensions is very similar to one in three dimensions. He photographed a close-packed random layer of particles; chose one as center and drew concentric circles round this one; and by counting the number of particles between circles derived the density function. A one layer technique can be used to find W. If two particles are marked the measured distance between these two particles will give values of r. The particle array is changed by shaking the container. This technique is applicable to actual clastic sediments provided that the particles are relatively large. In one or two dimensions Monte Carlo methods can be applied using the random numbers supplied by statistical tables (Smalley, 1962). Placing random circles in a square frame has been found to give a maximum loose random packing density of about 0.6. It is necessary to distinguish between loose random packings and tight random packings. By random placement it is possible to obtain a random arrangement of circles that are packed tightly enough to allow no more to be added and yet have no contact. This would represent a maximum density loose random pack; a maximum density tight random pack would have maximum contact as well.

Thus the loose random pack in two dimensions has a similar density to the tight random pack in three dimensions.

THE RADIAL DISTRIBUTION OF EQUAL SPHERES IN A RANDOM AGGREGATE

Scott (1962) has used a very elegant technique to determine the radial distribution of random close-packed equal spheres. His results (fig. 3) give the most accurate representation of the structure of a random sphere pack. About 4000 steel balls produced the pack, which was then set with wax. The outside layers were removed, and the coordinates of the inner spheres determined by an optical comparator. The positions of about 1000 balls were measured, arbitrary centers were chosen, and the interparticle distances were calculated by an IBM 650 computer. Twenty-five centers were used, and the value N_{av} represents the average number of spheres found at intervals of 0.2d: $N_{av}/4\pi r^2$ becomes constant for large values of r. Bernal, Mason, and Knight (1962) used a mechanical three-point contact device to measure the sphere position. This method would be applicable to a particle sediment provided that the particles were gravel size and preferably Zingg class II.

It may be that all clastic sediments have very similar radial distributions but it seems probable that certain cases will show unusual structures. Markedly bimodal sediments like certain coarse alluvial deposits which are geometrically far removed from collections of uniform spheres of equal size could have un-

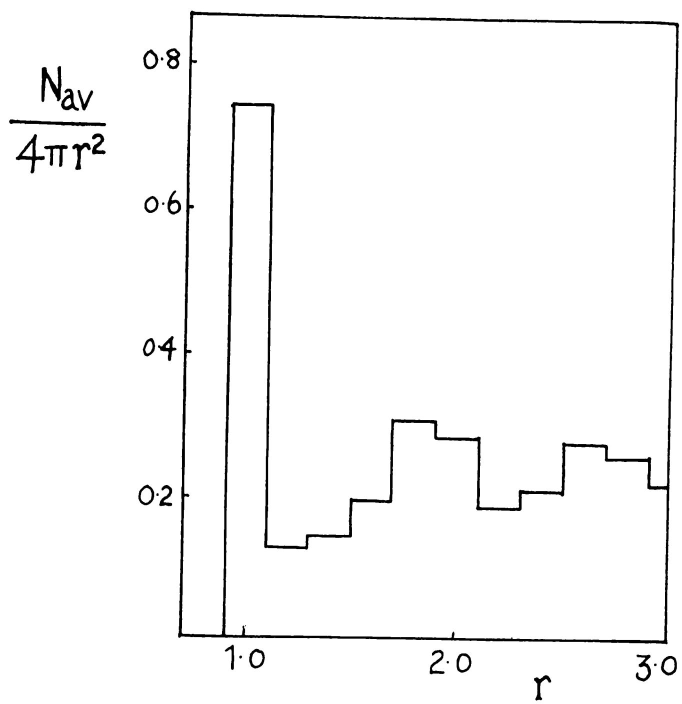

Fig. 3. Histogram at intervals of 0.2d of $N_{av}/4\pi r^2$ against r. N_{av} is the number of particles at distance r from an arbitrary center.

usual radial distributions because the smaller particles can occupy the spaces between the large ones. This is a basic problem: in what way does the range in particle size in a clastic sediment affect the structure? The effect on the density of a range of particle size has been investigated by Yerazunis, Bartlett, and Nissan (1962). They found that in a binary mixture of spheres with diameter ratio 1:3.8 there is a range in density from 0.63 to 0.69. The maximum density occurs when the large spheres form 60 percent of the pack. Since the change in density is only of the order of 10 percent it seems unlikely that the variation in structure is very great. With a diameter ratio of 1:47 the increase in density is greater but with this large difference in size it is likely that the large particles form random structure and the smaller ones fill the spaces. This size distribution is not one which would occur in a natural clastic sediment. It appears that only certain diameter ratios will have an appreciable effect on the structure. An attempt to generalize the relationship between density and diameter ratio has been made by Epstein and Young (1962).

The radial distribution function variation gives a better representation of the packing of the particles in a clastic sediment than a regular unit cell or mixture of cells. It is to be hoped that as in the case of liquids the definition of the structure will lead to some useful rationalizations about the properties.

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