Densification by the successive crushing of grains

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ABSTRACT: Discrete element methods have been widely used to investigate the behaviour of assemblies of granular materials under applied stresses and deformations. Usually the particles are represented by elliptical or ellipsoidal elements which may deform at contact points, but which are not permitted to fracture. McDowell, Bolton and Robertson[3] demonstrated some of the principles which could be used to explore the statistical fracture mechanics of a granular aggregate. An iterative scheme is used in which particles, represented by rigid, close-packed, triangular elements are assigned finite probabilities of fracturing. The probabilities depend on the value of increasing macroscopic stress, particle size and co-ordination number. No attempt is made to assess local equilibrium or to include contact deformations. This earlier work is now extended to include the explicit presence of voids. As stress increases, particles begin to fracture and a kinematic rule permits broken fragments to fall, so that the voids ratio reduces. The forms of the derived plots of voids ratio against the logarithm of the macroscopic stress are discussed.

INTRODUCTION

McDowell, Bolton and Robertson[3] (1996) introduces a two-dimensional numerical model, using an extension of Weibull statistics, in which a granular medium under stress evolves as a function of the behaviour of individual grains. An initial sample of uniformly sized grains is represented by an array of identical right-angled triangles, each of which might fracture to create two right-angled triangles in its place. Starting from an initial level of macroscopic stress a pass is made of the triangles, fracturing them on the basis of the proposed probability equation. When a sufficiently small proportion of the triangles fracture during a single pass, the level of stress is increased and the process repeated. For each increment of stress the corresponding reduction of voids is deduced from the amount of breakage occurring, using a work equation. A simulated compression curve is generated, showing the voids ratio versus the logarithm of the macroscopic stress. In this case, however, the voids are not explicit in the geometry of the aggregate.

Earlier work has referred to the fractal nature of a debris of crushed fragments (Sammis, King and Beigel[5] (1987); Palmer and Sanderson[4] (1991); Turcotte[6] (1996)). Bolton and McDowell[1] (1996) advance the hypothesis that both sands and clays adopt such a fractal geometry on their "normal consolidation line" and propose mechanisms of "clastic yielding" followed by "clastic hardening". Clastic yielding is the onset of fracture of the weakest particles of the aggregate. Clastic hardening occurs because the fracture strength of the broken fragments exceeds that of their progenitors. Self-similarity can emerge in the hardening, crushing aggregate, and particle size distributions can display some fractal properties.

The new simulation first creates a "loose" assembly of triangles with voids, and the migration of fragments. The resulting compression curve is therefore solely a function of statistics and kinematics.

INITIALISATION - CREATING A SAMPLE

The purpose of the initialisation process is to generate an initially stable assembly of equally sized, triangular elements, containing voids, so that the reduction of these voids within a region can be observed when a fracturing process is introduced. In reference to the sample, the terms "porosity" and "void ratio" of a region are taken to mean the proportion of area not covered by any triangle, and the ratio of the areas of voids and triangles. As a first step, a solid array of 200 triangles containing no voids is created (e.g. Fig. 1)

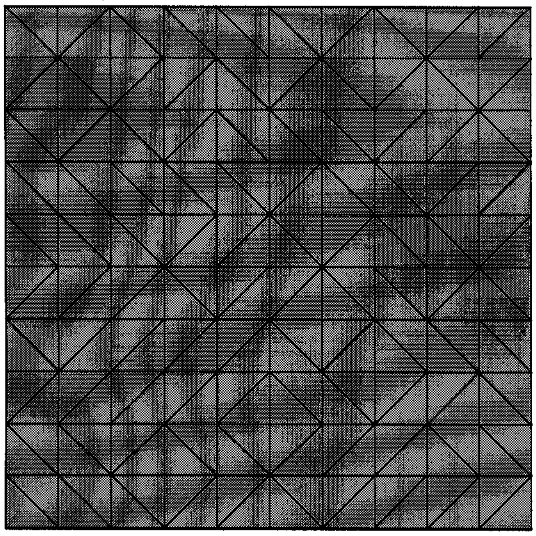

Fig. 1 - Solid array of triangles.

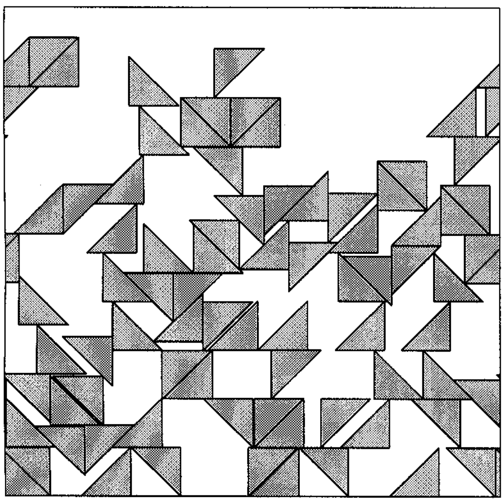

Fig. 2 - Generation of "initial" sample.

Particle removal and filling

Particles are next removed, one at a time, opening up voids within the sample. Each particle in the current sample has an equal probability of being removed. Following each removal, the remaining particles are permitted to fall and slide according to simple kinematic rules, so that some of the space created migrates towards the top of the sample.

Whenever a sufficient amount of space becomes available at the top of the sample, a fresh block of 20 triangles is introduced and allowed to fall, to replenish those which have been removed.

The aim is to repeat this process a sufficient number of times until a region has been formed within the sample in which the density of the triangles might acceptably be described as "loose" (e.g. Fig. 2).

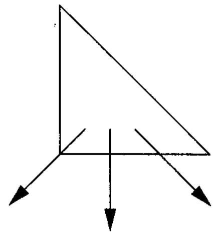

Fig. 3 - Direction in which particles may fall.

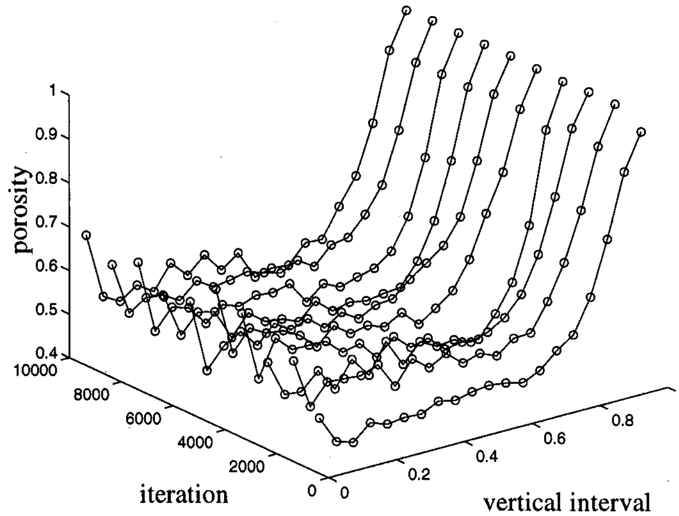

Fig. 4 - Average porosity.

Kinematics

Triangles are not allowed to rotate and are permitted to fall in only three directions: vertically, or downwards at an angle of 45 degrees (Fig. 3). Triangles may fall whenever their movement in a particular direction is not blocked by another particle.

A horizontal "wrap-around" is implemented so that particles which fall out or protrude from one side of the sample are allowed to fall in or intrude into the other side. This wrap-around is taken into account when the co-ordination numbers of particles is being calculated. No corresponding vertical "wrap-around" is defined. Particles which come into contact with the base of the sample are not permitted to fall further.

A triangle which is able to move, moves according to the following rules. First, the particle is allowed to fall as far vertically as it can until it comes into contact with another triangle or reaches the base of the sample. Assuming it has not reached the base of the sample, it is then allowed to fall in one of the diagonal directions, selected at random, until it again comes into contact with another triangle or reaches the base of the sample. If the triangle is unable to move any distance in the diagonal direction selected, then it is allowed to fall as far as it can in the other diagonal direction. Having now fallen diagonally, the triangle is again permitted to fall as far vertically as it can and the process repeated until the triangle is no longer able to move, being constrained in the three possible directions by other triangles or the base of the sample.

For the purposes of determining how far a triangle may move, or with which other triangle it is in contact, the sample space is considered to be divided into a grid. Each triangle maintains a list of the boxes of the grid which it overlaps and each box maintains a list of the triangles by which it is overlapped. The grid is chosen so that the width of its squares are slightly larger than the size of the initial triangles so that each triangle need maintain at most 4 boxes in its list. In calculating the co-ordination number of a triangle, only the triangles belonging to these boxes need be examined. Triangles which share more than one box are counted only once.

A triangle may be prevented from moving in one of the directions by more than one triangle. However, to simplify storage, each triangle stores the identities of one constraining triangle for each of the three directions. These are updated whenever a triangle falls, or attempts to fall.

If a triangle falls, or is fractured, or is removed, a pass is made through those triangles with which it previously shared a box. Those which had recorded the triangle as a constraint are appended to a list of potentially unstable triangles. Each triangle on this list is then considered in turn and tested to determine whether it can now fall. If it is still prevented from moving, its constraints are updated and it is removed from the list, otherwise it is allowed to fall. This may or may not result more triangles being appended to the list. When all triangles have been removed from the list, every triangle in the sample is again constrained in each direction. When a triangle splits, the resulting fragments are automatically appended to the list of potentially unstable triangles.

The boxes are also used when determining the maximum distance a triangle may fall in a given direction. The distance is initially set to the that required for the triangle to come into contact with the base of the sample. Starting form those boxes to which a triangle currently belongs, those boxes which might contain an intervening triangle are then considered in turn. The triangle is tested against all of the triangles belonging to the current box. This is continued until the maximum distance found is zero, or less than the distances to the boxes still to be considered.

Statistics/Sampling

Initially, as triangles are removed from the sample the overall density of triangles decreases.

The voids ratio calculated during the fracturing process is based on a sub-sample within the assembly of triangles created during the initialisation process. The proportion of area occupied with triangles is considered within 20 equally sized horizontal layers through the sample. Fig. 4 shows the porosity of the 20 layers averaged out over periods of 1000 iterations within an initialisation period of 10,000 iterations. From this graph, and the trend and scatter from each successive iteration a sub-sample was chosen extending from 10% to 60% of the total height of the sample, from the base.

An initialisation period of 1,000 iterations was found to be sufficient to ensure that the assembly of triangles was sufficiently random. In general, the porosity in the sub-sample rises rapidly to a reasonably stable level long before this.

Once a "loose" sample has been generated in this way, the fracturing process is applied.

STATISTICS OF FRACTURE OF A GRAIN

The model for breakage is based on Weibull[7] statistics of failure. Weibull postulated that the probability of the survival of a specimen, of a given size, subjected to a tensile stress σ could be written in the form:

$$P_s(\sigma) = exp\left\{-\left(\frac{\sigma}{\sigma_0}\right)^m\right\} \tag{1}$$

where m, the Weibull modulus, is a measure of the variability in the strength of the material, increasing with decreasing variability, and σ_0 is the value of stress at which approximately 37% of the samples survive (Fig. 5).

Weibull also recognises that the survival of a block of material under tension requires that all its constituent parts remain intact. The mean fracture strength decreases as the size of the specimen increases. For a block of material of volume V, under an applied tensile stress σ, the survival probability of the block is given by:

$$P_s(V) = exp\left\{-\frac{V}{V_0}\left(\frac{\sigma}{\sigma_0}\right)^m\right\} \tag{2}$$

McDowell, Bolton and Robertson[3] used a modified survival equation which introduces an extra term to account for the variable co-ordination number of the particles, and so that the maximum tensile stress induced within a particle reduces as the number of contacts increases. The survival probability of a 2D grain is then given by

$$P_s(d) = exp\left\{-\left(\frac{d}{d_0}\right)^2\frac{(\bar{\sigma}/\sigma_0)^m}{(C-2)^a}\right\} \tag{3}$$

where d is the size of the particle, d_0 is the size of the original particles and the factor a can be used to vary the degree to which the co-ordination number C affects the probability of fracture.

The same equation is used in this simulation. In the original work no triangles were allowed to move and the co-ordination number was taken as the number of triangles sharing an edge. The minimum possible co-ordination number was therefore 3. Here the particles may move and for ease of calculation the co-ordination number is taken to be the number of triangles sharing any contact: edge-to-edge, edge-to-corner or corner-to-corner. Two triangles are considered to be in contact if the distance between them is below a very small tolerance value, based on the size of the smaller of the two triangles. Since it is now possible for a triangle to have only one or two neighbours, the value of C is arbitrarily set to a value of 10 in the probability equation if the particle has less than 3 neighbours, to give these particles a very small chance of fracturing.

COMPRESSION

McDowell, Bolton and Robertson[3] did not explicitly represent voids in the model. Fig. 6 shows the fractal geometry of the broken fragments after a significant increase in stress. It was argued that such a figure could be regarded as creating a logical map of co-ordination numbers and particle sizes. An implicit voids ratio e was then inferred by applying a work equation. The work done per unit volume by the macroscopic stress $\bar{\sigma}$ was written $\bar{\sigma}de/(1+e)$ and equated to the work absorbed in fracture and frictional rearrangement.

The following relationship was derived to calculate the change in voids ratio associated with each increment in stress:

$$\frac{de}{(1+e)} \propto \frac{\Gamma}{(1-\mu)\bar{\sigma}} \sum_{r=0}^{r=s} B_r d_r \qquad (4)$$

where the orders of the particle sizes are listed as r=0 for the largest particle (size d_0) and $r = s$ for the smallest (size d_s), and B_r is the number of particles of size d_r which are splitting. Γ is the critical strain energy release rate, a measure of the "material toughness", and μ is a function solely of the internal angle of friction.

In calculating the value of de in the simulation, equation 4 was simplified to:

$$de = \frac{K}{\bar{\sigma}} \sum_{r=0}^{r=s} B_r d_r \qquad (5)$$

where K is taken to be a constant.

Fig. 7 shows a simulated compression curve generated using this approach. In the current simulation the voids ratio is calculated directly from the area of triangles within the sub-sample rather than from the work equation.

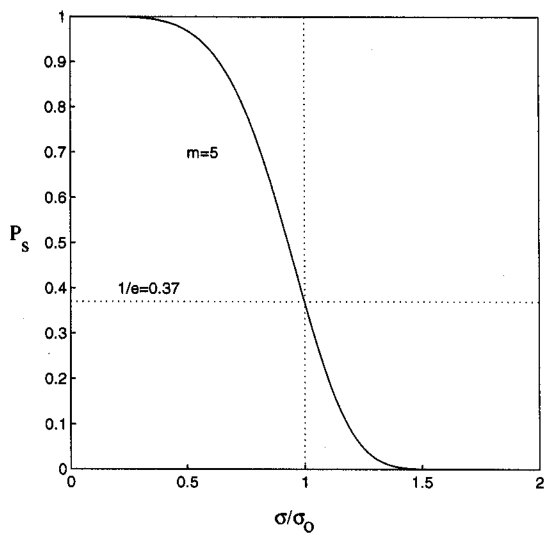

Fig. 5 - The Weibull function.

A stress level is initially calculated such that a single particle fractures. After each set of fractures the earlier kinematic rule, used to generate the initial sample, is invoked and the crushing and subsequent falling of particles is allowed to continue until less than 2% of particles fracture in a single pass of the triangles. The stress is then increased by 1% and the process continued.

Fig. 8 shows the sample after 1193 iterations and Fig. 9 shows the corresponding compression curve. The form of this curve differs from the curve generated using the work equation. During the first stages of fracturing the sample has undergone significant compression, corresponding to the fall in the first part of the compression curve. However, larger triangles with relatively large survival probabilities then begin to form a stable structure through which the smaller particles are unable to fall. Although fracturing continues to occur, the tendency is for the smaller particles to continue crushing and the curve begins to level out. The grading curve of the sub-sample, is shown in Fig. 10. Fig. 11 shows the porosity within 20 vertical slices through the entire sample space. This show the values within the chosen sub-sample to be reasonably consistent.

The statistical rules adopted in the new kinematic simulation lead to something of a paradox. Heavily fractured debris tends to continue crushing even though it appears to lie on the "floor" of a "cave" formed between larger blocks. The answer lies in relaxing the condition that all particles should carry a fair share of the macroscopic stress. The best way of achieving a lifelike soil structure, and a reasonable variation in local stress, is under investigation. The theoretical ideal would be to capture the detailed equilibrium and kinematics of every grain. This

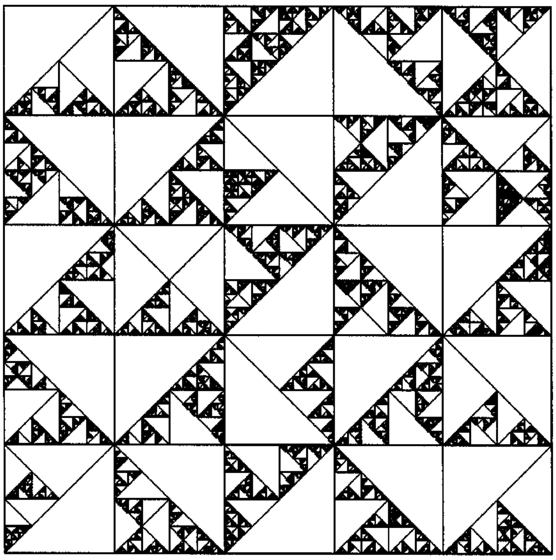

Fig. 6 - Fractal geometry for explicit voids.

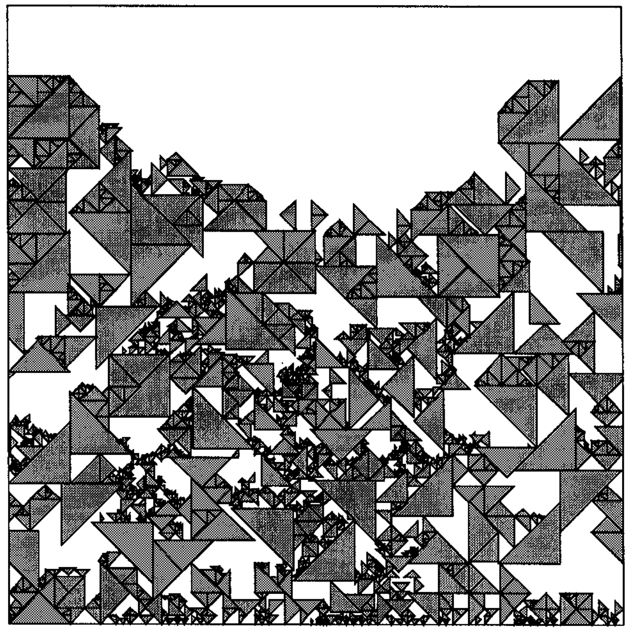

Fig. 8 - Sample containing 2083 triangles.

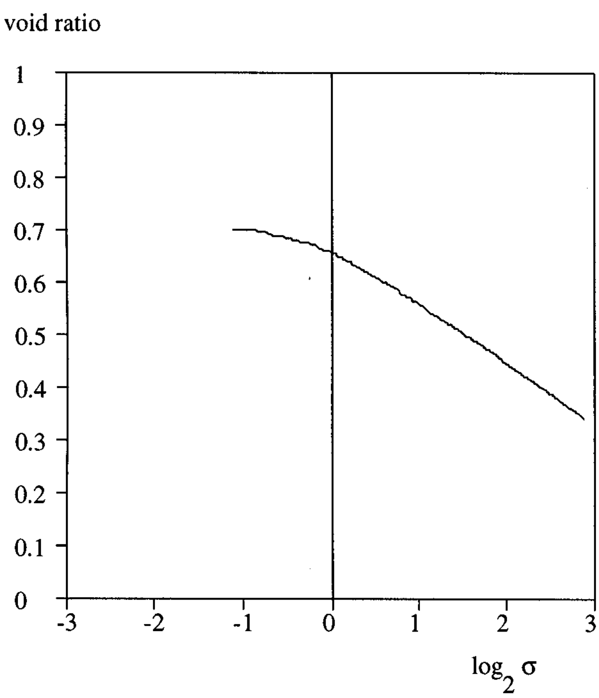

Fig. 7 - Compression curve using the work equation.

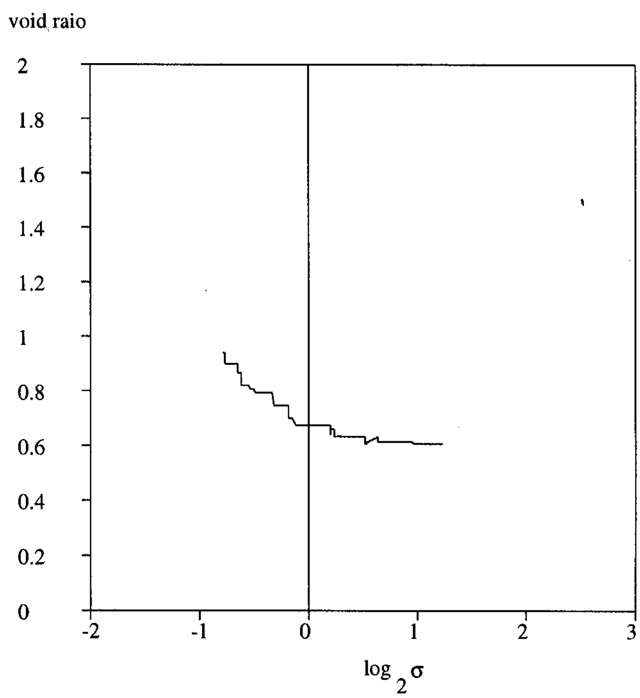

Fig. 9 - Compression curve calculated from area.

seems not to be a realistic computational proposition if, as proposed, the successive creation of many generations of fragments is an essential pre-requisite to the modelling of "plastic" compression in granular media. The statistical approach, adopted here, appears to have some promise.

CONCLUSIONS

1) Techniques are available to obtain simulated compression curves using statistics of fracture of rigid clasts.
2) Voids can be created by particle removal, and a statistically reliable "loose" soil can be generated.
3) Stress analysis and Weibull statistics lead to successive fracture, rearrangement, wide gradings, efficient packing, and the irrecoverable reduction of voids.
4) Work is in hand relating the kinematics of broken fragments to earlier observations of fractals, and the use of a work equation to derive changes of voids ratio.

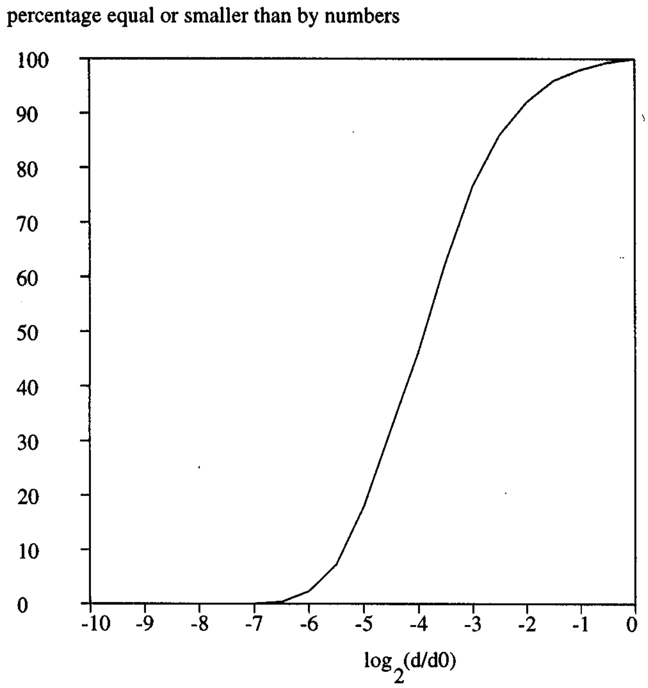

Fig. 10 - Distribution of particle sizes.

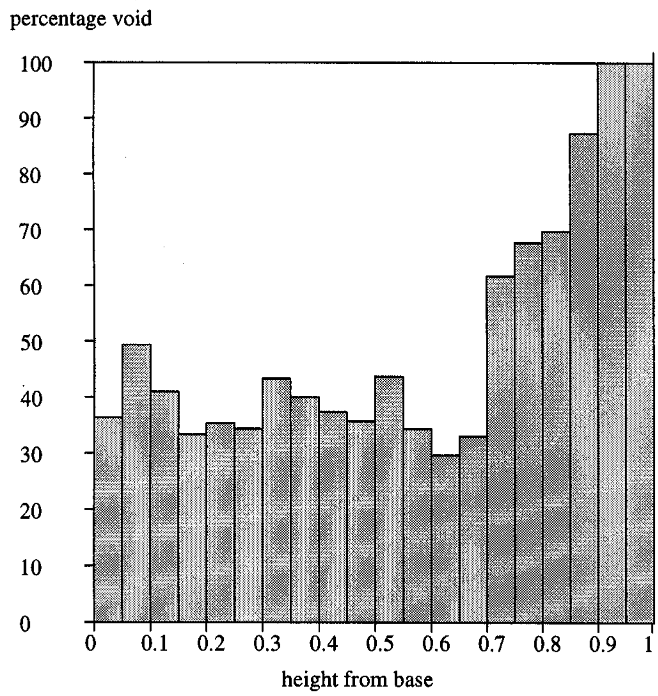

Fig. 11 - Porosity within vertical slices.

REFERENCES

1) M. D. Bolton and G. R. McDowell, 'Clastic Mechanics', *IUTAM Symposium on Mechanics of Granular and Porous Materials* (1996)(in press)
2) P. A. Cundall and O. D. L. Strack, 'A discrete numerical model for granular assemblies', *Geotechnique*, **29**, 47-65 (1979)
3) G. R. McDowell, M. D. Bolton and D. Robertson, 'The fractal crushing of granular materials', *Int. J. Mech. Phys. Solids.* **44**, 2079-2102 (1996)
4) A. C. Palmer and T. J. O. Sanderson, 'Fractal crushing of ice and brittle solids', *Proc. R. Soc. Lond. A* **433**, 469-477 (1991)
5) C. Sammis, G. King and R. Beigel, 'The kinematics of gouge deformation', *Pure Appl. Geophys.* **125** 777-812 (1987)
6) D. L. Turcotte, 'Fractals and fragmentation', *Journal of Geophysical Research* **91**, 1921-1926 (1986)
7) W. Weibull, 'A statistical distribution of wide applicability', *J. Appl. Mech.* **18**, 293-297 (1951)