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QUANTITATIVE DESCRIPTION OF STRUCTURAL CHANGES IN SOIL AND PLANT MATERIALS DURING DEFORMATION

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A b s t r a c t. A quantitative proposition for the description of structural changes in three-phase media was proposed. Random variables were used as representing the structure and its changes. The consequences for both: theoretical considerations and new experimental approach were demonstrated.

K e y w o r d s: three-phase media, probabilistic micromechanics, structure

INTRODUCTION

It is common that flows and deformations in agricultural materials are defined and measured on the surface of samples blocks or profiles. That is why during deformation or flow the structure and its changes are not considered and a 'black box model' can be proposed only.

The material is treated as homogeneous and continuous by experimentator and the changes of its structure during process are neglected. The non-linearity inherent in the structure of three-phase agricultural material cannot be introduced into theoretical considerations.

CONSEQUENCES OF DETERMINISTIC AND PROBABILISTIC METHODS IN THE MECHANICS OF THREE-PHASE MEDIA

Agricultural media are composed of three distinct phases: solid, liquid and gas. All these phases have an important contribution to the resulting flows and deformations, i.e.:

- solid phase creates a skeleton which causes that the medium behaves like a solid material and tends to keep its shape;
- liquid phase is responsible for a filtration effects, neutral stress and time dependent behaviour;
- gas phase makes a voluminal deformations (usually instantaneous and irreversible) possible, which in turn changes the structure during deformation considerably.

Comparing the existing theories of deformation and flow in three-phase media one can distinguish four methods at the very first point, i.e., at the moment of definition and measurement of gradients, stresses and strains (Table 1).

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Table 1. Possible methods in mechanics of three-phase media

Method	Definitions	Consequences
Deterministic approach	Continuous homogeneous medium, stresses and strains in the form of derivatives: $f = \lim_{\Delta S \to 0} \frac{\Delta F}{\Delta S}$, $D = \lim_{\Delta l \to 0} \frac{\Delta l}{lo}$, motion in 'ordinary' space x, y, z, t	Linear thermodynamics of irreversible processes, Onsager's recriprocal relations, linear physical (constitutive) equations - laws of heat and mass flow, elasto-visco-plasticity
Statistical approach	Discrete system of equal elements, stress and strain are sums for all elements: $f = n \frac{\Delta F}{\Delta S}$, $d = n \frac{\Delta l}{lo}$, motion in 'phase space' of generalized coordinates (p, q, t)	Statistical thermodynamics, ergodic theorem, non-linear statistical constitutive theory, non-linear flow, non-linear elasto-visco-plasticity
Probabilistic approach	Discontinuous unequal structural elements, integral stress and strain: $f = \int \frac{\partial F}{\partial S} dF$, $d = \int \frac{dl}{l}$ 'motion' in the space of random variables (obtained experimentally)	Probabilistic theory formulated 'from the first principles' (formulated for one structural element - pore, grain, cell - and then integrated for the whole structure), deterministic final equations
Stochastic approach	Measurable output signals and non-measurable 'white noise of background', discontinuous structure, integral stress and strain	Stochastic processes, probabilistic final equations (probability of transition between states)

Traditionally the first approach for the prediction of the response behaviour have been used, which is based on the continuum theory. This method refers to the homogeneous media, ignoring thereby the presence of the microstructure of medium. The stress and strain involved in the formulation of the main objective that govern the mechanical response of a given material under given specific environmental conditions are introduced as an infinitesimaly small derivatives and differentials. Then linear relations between forces and deformations or flows are formulated.

As it was shown [2-5] this theory is valid so far as the linear thermodynamics of irreversible processes together with the Onsager's relations are valid. Additional latent conditions have to be fulfilled (e.g., flows have to be laminar, potentials - parabolic, deformations and gradients - mathematically small together with their time derivatives).

When the structure can be well approximated by the system of equal elements (like in crystals, liquids and gases), it is possible to use statistical thermodynamics - second approach. These enable to define stresses and strains as the multiplication of effect for single element by the number of elements and to get some non-linear physical laws (constitutive equations).

Probabilistic micromechanics (the third approach) is concerned with the formulation of the stress-strain response but with the inclusion of the microstructural effects that are due to the inherent geometrical and physical properties of structured three-phase media. Method of stochastic processes is even 'more statistical' in the meaning that not only the state of the medium, but the physical relations (governing equations) are probabilistic as well. It is obtained using the probabilistic theory of transition of the system between subsequent states defined by the different values of the deterministic and random variables of state (e.g. theory of Markov processes).

QUANTITATIVE DESCRIPTION OF THE SOIL STRUCTURE USING RANDOM VARIABLES

Most of the significant field quantities involved in any formulation of the material behaviour are by nature random variables or functions of such variables. They have to be determined experimentally. The structure is considered quantitatively using random variables, the values of which are related to the geometry and strength of a considered materials (grains, pores, aggregates, cells, fibres, etc.).

To show this we will consider the soil compaction case. We propose that the soil structure is described by four random variables the values of which are:

- grain and aggregate size distribution $g_1(Ds)$, which describes structure of solid phase;
- pore maximal diameter distribution $g_3(Dp)$, deciding which soil grains or aggregates can enter into a given pore during deformation;
- pore volume distribution $g_4(Vp)$, informing about the soil volume which can enter into a considered pore;
- distribution of contact forces $g_2(f)$, responsible for the stress inhomogeneities.

Let us estimate the density of random variable, the values of which are the diameters of particles and aggregates in the ivestigated soil (Fig. 1). Hereafter we will use the name 'grain' in the meaning of both: elementary soil particles and aggregates (unless the latter are destructed). We participate the set of values of diameters into intervals I_1, I_2, ...I_n. The participation follows from the used method of measurement of the grain size distribution and the greater number of intervals the better description. We assume that in each interval our random variable is uniformly distributed. Hence we obtain as an estimator of density the following function:

$$g_1(Ds) = \sum_{k=1}^{m} \frac{n_k}{N} \frac{1}{|I_k|} J_{[I_k]}(Ds) \quad (1)$$

where $|I_k|$ is the length of interval, N - number of all grains in the sample and

$$J_{[I_k]} = \begin{cases} 1, Ds \in I_k \\ 0, Ds \notin I_k \end{cases} . \quad (2)$$

We will now introduce the second random variable (random vector) which describes the pore diameter and length distribution. Analogously as with the density of grain diameter we estimate the density of this vector. Let us put that for a fixed pore diameter Dp the density of the random variable representing the pore length is estimated by:

$$g_3^{Dp}(Vp) = \sum_{j=1}^{m} \frac{n_j}{N} \frac{1}{|II_j|} J_{[II_j]}(Vp) . \quad (3)$$

This is the first component for the random vector (Dp, Vp) whereas the second component is given by the density:

$$g_4(Dp) = \sum_{i=1}^{m} \frac{n_i}{N} \frac{1}{|II_i|} J_{[II_i]}(Dp) . \quad (4)$$

In the above relations we have used the analogous notation as in the Eq. (1).

Hence we obtain the following estimator for the density of the considered random vector which describes the two-parametric pore size distribution:

$$g_5 = (Dp, V_p) = g_4(Dp)\, g_3^{Dp}(Vp) . \quad (5)$$

Let F_o denotes the mean external force on the soil surface, which is assumed to be the same in all directions for simplicity. The mean force in the contact point of any two grains is [4]:

$$f_m{}' = \left(\frac{18 F_o}{\pi (EDs)^1 (1+p_{min})} \right)^{2/3} \quad (6)$$

where $E\ Ds$ is the mean diameter of soil grain (aggregate) and p_{min} - the minimal final microporosity. The latter can be calculated from the experimental characteristics in the following way:

The volume of the measured pores (e.g. bigger than 0.2 μm in diameter) is substracted from the soil volume and the calculated porosity of a rest soil 'matrix' is defined to

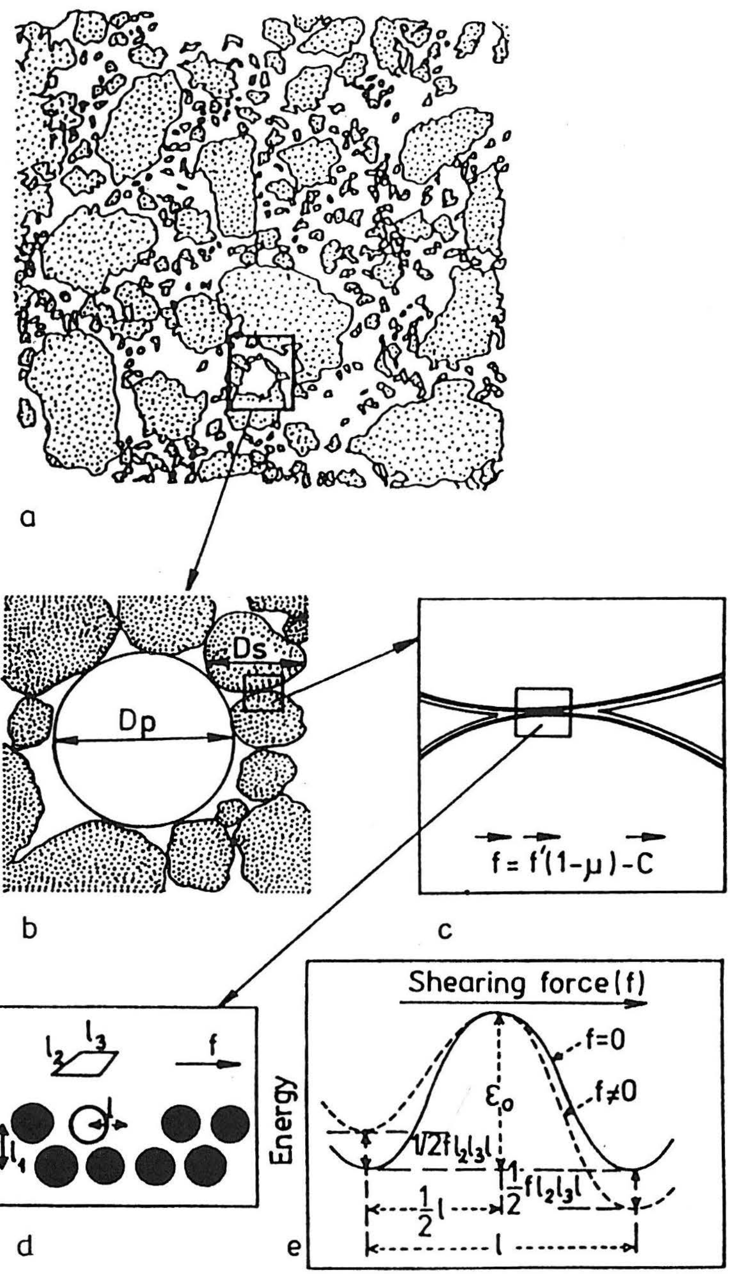

Fig. 1. Cross section through a sample of loess and qualitative description of its structure: a - sample cross section, b - pore cross section (Ds - grain diameter, Dp - pore diameter), c - contact of grains (f' - external force), d - molecular layers (l_1, l_2, l_3, - molecular distances), e - energy barrier (Eqs (9) and (10)).

be p_{min}. As it was shown in [4], this porosity is almost constant for a given external stress F_o versus time. This means that we can imagine soil as a 'Swiss Cheese':

$$\text{soil} = \text{measured pores} + \text{soil with micropores.} \tag{7}$$

Only the first term in the right hand side of the above equation is changing for a constant external stress and it is responsible for the compaction effect, whereas the second term is increasing with the increasing stress walue.

There is no possibility of measurement of the intergranular forces and contact surfaces at present, as the size of the soil grains and aggregates changes within the range from some tenth of micron to centimetres and even decimetres for clods. However, one can see that this forces are fairly different in the experiment reported by Drescher [1], (Fig. 2).

The circles represent pills (cylinders) made of elasto-optical material placed between two horizontal glass plates in a plane stress state. Forces between pills were determined from the interference pattern in polarized light. The direction of lines between centres of circles represent the direction of forces, whereas their thickness - the value of this forces. One can see, how hardly this forces can be assumed parallel and equal.

MOTION OF SOIL GRAINS INTO A FIXED PORE

We will regard the force causing the viscous (time-dependent) motion of the grain as the difference between the external force f and the intergranular dry friction μf together with the cohesion C (Fig. 1):

$$f = f\,(1-\mu) - C. \tag{8}$$

Dry friction depends on the resultant force perpendicular to the direction of motion,

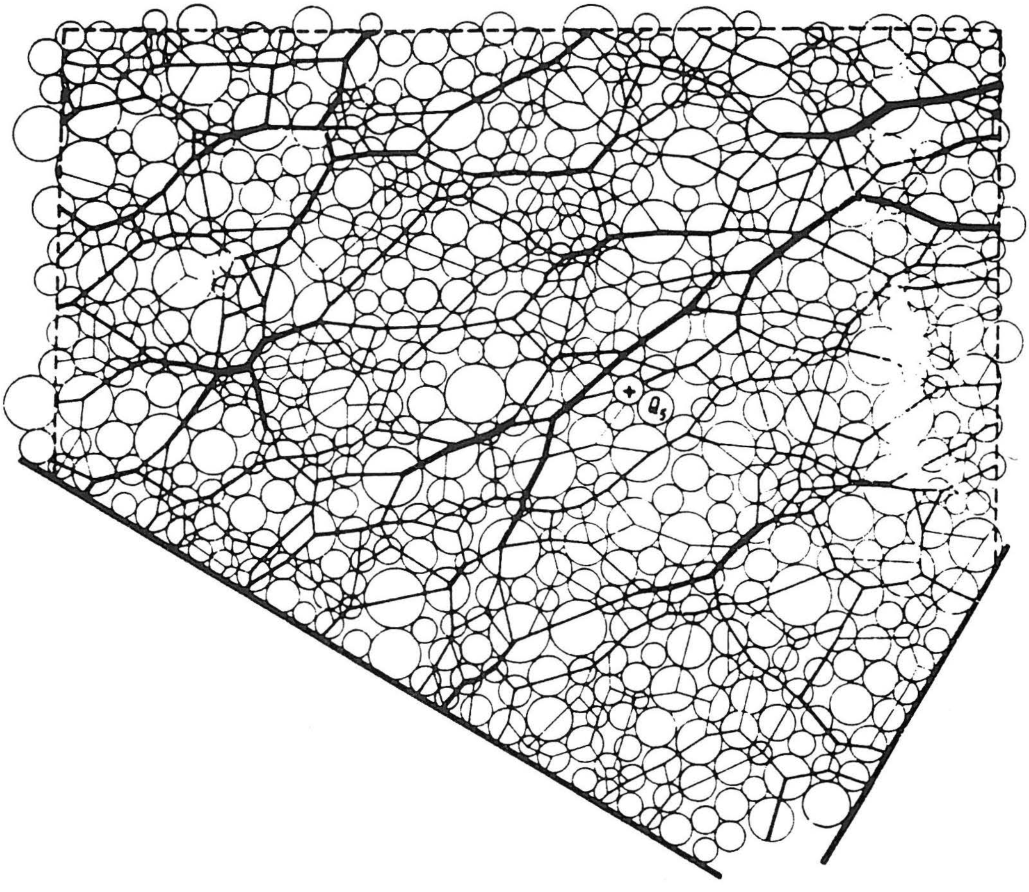

Fig. 2. Photoelastic vizualization of intergranular forces after Drescher [1].

viscous friction - on the tangent resultant force and cohesion is represented by the constant mean value.

For the mathematical simplicity we are assuming that the forces are equal in all directions without lost of generalization. It can be easily written in three-dimensional vectorial or tensorial representation. Applying the theorem about distribution of function of random variable the density of f is obtained in the form:

$$g_2(f) = g_2\left(\frac{f}{1-\mu} + \frac{C}{1-\mu}\right)\frac{1}{|1-\mu|}. \quad (9)$$

We will understand, that the negative value of f means that such stress does not cause any displacement. As one can calculate the probability of such event is of the order of 10^{-25} for typical soils. That is why instantaneous deformations are mostly irreversible, which could not be explained by any theory of visco-elasto-plasticity.

From physical considerations and experimental results presented in papers [2-5] we will assume the equation of motion of a soil grain into the pore in the form:

$$X = A \exp(Bf)\, t \quad (10)$$

where X is the grain displacement, A, B - constants of statistical non-linear viscous motion dependent on soil structure - especially water, clay and humus content, and t denotes time. Hence we have the analytical condition for the entrance of a soil grain into a pore:

$$A \exp(Bf)\, t > 0. \quad (11)$$

This condition gives us the lower boundary for the set of stresses causing the compaction:

$$h(A, B, t) = \max\left\{\frac{-\ln At}{B}, 0\right\}. \quad (12)$$

The function $h(A,B,t)$ implies the following fact. There exists t_{stop} such that the compaction stops for a given stress and that time t_{stop} is independent on stress. This is the crucial effect for both: verification of the new micromechanics of soil and practice.

In order to express the probability of the event that the soil grain gets into a pore we need the following preparations:

- it is natural to assume that the size distribution of grains belonging to the 'pore surface' is the same as that in the whole sample;
- it is also natural to assume that the grain cannot enter into a pore when its diameter is higher in value than that of the considered pore;
- it is well known and established in many experiments that the larger pores are more susceptible for the destruction during deformation. To take it into consideration qualitatively we will propose that the probability of grain motion into a pore described by the parameters (Dp,Vp) is proportional to (Dp, Vp).

The latter assumption means that the strength of a pore decreases proportionally to its maximal cross section or 'surface', which one can imagine as the force flux in the pore.

Let D stands for a random variable the values of which are the diameters of particles entering into a pore. The random variable can have 'mass at 0 point', i.e.,

$$P\{D = 0\} \geq 0 \quad (13)$$

which means that there is no grain entering into a pore. D can take the other values, which belong to the interval (Ds_{min}, Dp). In this interval D appears to be a continuous variable with the density:

$$g_6(Ds, Dp, Vp, Vp, f, t) =$$

$$DpVp\, g_1(Ds)\, c_3(f_m)$$

$$\int_{h(A,B,t)}^{2f_m} g_2(f)\, df \quad (14)$$

where Dp, Vp, t are parameters, f is defined above and C_3 depends on f_m.

THEOREM ABOUT THE NORMAL DISTRIBUTION OF SOIL COMPACTION

For every soil grain moving into a pore we construct a random variable the value of which is its diameter *Ds*. These random variables are independent and identically distributed as *D* which means that the grains appear independently into a pore. It is to be stressed that we are considering one pore with the fixed parameters *Dp*, *Vp* for a constant mean stress f_m.

Knowing the diameter of grain we can determine the value of its volume. Applying the forementioned theorem about the distribution of function of random variable, the distribution of a new random variable *V(Dp,Vp)* can be obtained. This variable takes values equal to the volume of grains entering into the pore. The same consideration as for the grain diameter gives us a set of random variables describing the volume of entering grains. The random variables *D* are independent and identically distributed also.

In order to express the final volume occupied by soil grains in the pore we will now determine the number of grains which are able to get it. It is the number denoted by *N(Dp, Vp)*:

$$N(Dp,Vp) = \left[\frac{Vp}{V_{EDs}}(1-p_{min})\right] \quad (15)$$

where *Vp* is the volume of the pore, V_{EDs} - the volume of the mean grain, p_{min} - the minimal final porosity of the compacted soil with micropores (Eq. (7)) and the square bracket [ ] stands for the Entire function.

It is obvious that the minimal porosity p_{min} decreases with the increasing force f_m and it can be measured from the pore size distribution.

Let V_i be a sequence of independent identically distributed random variables and let *V* has the same distribution function as *Vp*. The random variable defined by:

$$S_{N(Dp,Vp)} = V_1 + V_2 + \ldots + V_n$$

describes the final volume occupied by the soil grains in the fixed pore (*Dp*, *Vp*) for the constant mean force f_m. Using the central limit theorem [5] one can prove that $S_{N(Dp,Vp)}$ is asymptotically normal distribution (*N*):

$$S_{N(Dp,Vp)} = N\left(ES_{N(Dp,Vp)}, \sigma S_{N(Dp,Vp)}\right). \quad (16)$$

Usually it is assumed that the intergranular stresses or displacement are asymptotically normal distributions. We have proved that the sum of the soil volumes entering into a fixed pore can be approximated by normal distribution, which is very usefull for further statistical considerations.

EQUATION FOR ALL PORES AND GRAINS

We have investigated the voluminal changes in one pore as dependent on the four independent random variables describing the soil structure (*Ds*, *Dp*, *Vp*, *f*), time *t*, as well as the mechanism of dry and viscous friction (*A*, *B*, *u*, *C*).

We can calculate now which part of the volume of the pore (*Dp*, *Vp*) is filled with the soil grains. From the Eq. (16) we obtain the mean volume of particles which entered into this pore in the time *t* for the fixed mean force f_m:

$$ES_{N(Dp,Vp)} = N(\bar{D}p,\bar{V}p)\, EV(Dp,Vp)Dp \cdot lc_3(f_m) \int_{h(A,B,t)}^{2f_m} g_2(f)\, df. \quad (17)$$

We have used Eq. (14) and the term *N(Dp, Vp)* was substituted by its value for the mean diameter $\bar{D}p$ and mean volume $\bar{V}p$ and the mean volume of the pore equals:

$$E\,[V(Dp,Vp)] = \frac{\pi}{6} \int_{Ds_{min}}^{Dp} (Ds)^3\, g_1(Ds)\, d(Ds). \quad (18)$$

We can calculate now which part of the pore (*Dp*,*Vp*) was filled by grains during the time *t*:

$$V_t^{Dp,VP} = \frac{N(\bar{D}p, \bar{V}p)\, E[V(Dp,Vp)]\, D_p}{\left(\frac{\pi}{4} Dp\right)^2 l}$$

$$\frac{l c_3(f_m) \int_{h(A,B,t)}^{2f_m} g_2(f)\, df}{\left(\frac{\pi}{4} Dp\right)^2 l} =$$

$$= \frac{2}{3} \frac{N(\bar{D}p,\bar{V}p)\, E[V(Dp,Vp)]}{Dp}$$

$$c_3(f_m) \int_{h(A,B,t)}^{2f_m} g_2(f)\, df. \qquad (19)$$

To construct the process for all pores (Fig. 3) we have to take initial volumes for all pore fractions from the experiment [5] and to integrate the equations for all distributions: grain diameters, pore diameters and volumes as well as for all intergranular forces. We will limit our calculations for the diameters higher than 0.2 um which is justified by some experiments [5] and gives a reasonable simplification of calculations.

Roughly speaking V_{0k} denotes the initial total volume of all pores such that $Dp \in II_{0k}$. The fraction

$$\frac{S_{N(Dp,Vp)}}{Vp} \qquad (20)$$

determines which part of the pore volume has been filled. Combining this with the pore distribution expressed by the density $g_5(Dp, Vp)$ and the initial volume of fraction V_{0k} and integrating for all distributions of random variables we obtain the following equation for the mean pore volume filled by the grains in time t:

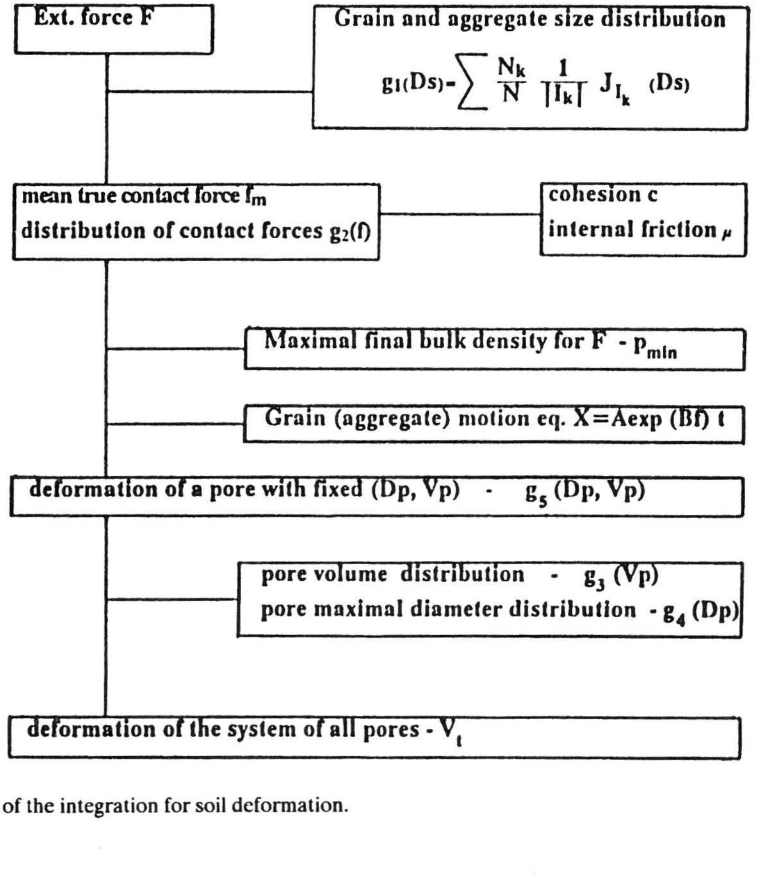

Fig. 3. Scheme of the integration for soil deformation.

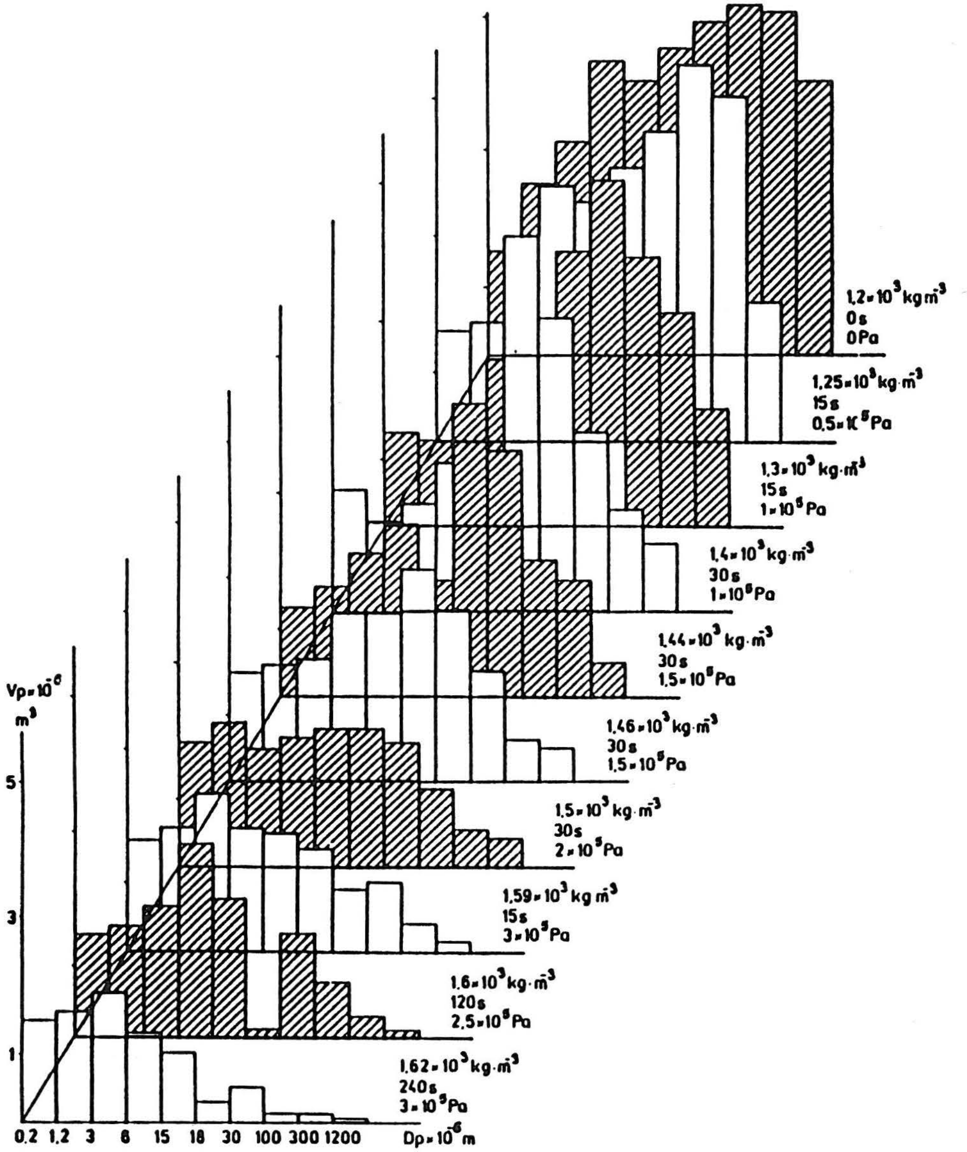

Fig. 4. Pore diameter distributions for loamy soil versus stress and time.

$$Vt = \sum_{k=0}^{n} V_{0k} \frac{2}{3} \left[\frac{\bar{V}pk}{EDs} (1-p_{\min}) \right] \int_{Dp \in II_k} \frac{\int_{Ds_{\min}}^{\min(Dp, Ds_{\max})} (Ds)^3 g_1 (Ds)\, d(Ds)}{Dp} \cdot$$

$$c_3 (f_m) \int_{h(A,B,t)}^{2f_m} g_2(f)\, df \cdot \qquad g_4 (Dp) \frac{N_p}{N_k} \qquad (21)$$

where $C_3(f_m)$ is the constant of normalization which can be calculated from the condition:

$$\int g_2(f)\, df \to 1 \text{ when } t \to \infty .$$

It has the form:

$$c_3(f_m) = \frac{Vt}{\sum_{k=1}^{n} V_{0k} \left[\frac{\bar{V}_{pk}}{EDs} (1-p_{min}) \right]}$$

$$\frac{Vt}{\int_{Dp \in II_k} \frac{E\, V(Dp,J)}{Dp}\, g_4(dp)\, d(dp) \frac{N_p}{N_k}} . \quad (22)$$

In this equation N_k is the number of grains entering into the 'mean' pore from the k-th fraction of pores. The difference between the total initial pore volume V_{0k} and the total final pore volume is the measured change of the sample volume V_t.

The final equation was compared with experimental characteristics for several soils (Fig. 4) with a good agreement.

Similar considerations are made for the deformation of plant cellular or fibrous material. In this case the structure is described quantitatively by random variables the values of which are sizes related with the cell or fibres properties respectively.

CONCLUSIONS

It is no accident then that the classical mechanics has not been able to establish a functional formulation of physical relations (constitutive equations) and, in order to obtain their linearity it has restricted itself to formulate local relations (linear theories of plasticity and viscoelasticity, linear laws of diffusion, water flow, heat flow).

To recognize the structure of the three-phase agricultural materials it is necessary to introduce an integral condition between forces and flows or deformations respectively together with a quantitative measure of structure in the form of random variables.

As it was shown in [2,4], the probabilistic equations obtained in this way can be reduced to the deterministic non-linear relations, which can be further reduced to the linear equations for small gradients, deformations, flows and their time derivatives.

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