SIMULATION OF STATISTICAL PACKINGS OF SPHERICAL PARTICLES

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UDC 519.6:539.215.4

An algorithm has been developed which simulates the process of statistically filling a fixed volume with spherical particles and which allows one to obtain the distributions of the coordination numbers of particles depending on the packing density.

The invention of composite materials on the basis of disperse systems and the mathematical description of their properties require the solution of the problem of determining the geometrical parameters of a packing of particles. One of these parameters is the coordination number which can be used for describing the strength of porous bodies [1]. Mathematical relations are available that couple the mean coordination number and the porosity of randomly packed spherical particles. However, until very recently no mathematical method was available which would allow one to obtain the distribution of the coordination numbers as a function of the packing porosity.

To solve the given problem, the evolution of the process of filling a fixed volume with spherical monodisperse particles under the action of gravity and vibration was simulated. Vibration is employed to obtain configurations with small enough porosities. The mathematical model is based on the method of particles [2]. To each particle there corresponds a set of coordinates in the three-dimensional space and the gravity force. The input data are the size of particles, volumetric filling of the system, and the magnitude of the time step. The motion of each particle depends on the location of surrounding particles.

Initially the particles are located at the nodes of a face-centered lattice at distances corresponding to a given volumetric filling:

$$h = 2r[\sqrt[3]{\varphi/\varphi_m}/(1 - \sqrt[3]{\varphi/\varphi_m})],$$

φ_m is taken to be equal to 0.64 [3]. The gravity force is applied along the axis Z. The particles are subjected to vibration along the axes X and Y. The approach selected ensures compaction of the packing of particles with time.

An algorithm which describes the sagging of particles under gravity and vibration is organized as follows. At the first stage the maximum displacement of particles in plane XY (the maximum amplitude of vibration) is calculated. It is governed by the arrangement of particles directly surrounding the particle considered. The maximum displacement along the axis (X or Y) is determined so as to prevent the moving particle from running into the neighboring one. The particle moves along the axis in one of the two directions corresponding to the maximum (for the given axis) displacement which does not allow the particle to strike the neighboring particles. The direct magnitude of displacement for each axis is selected randomly from the range limited by the maximum displacement found earlier. When vibration is taken into account, the particle moves successively first along the X and then Y axis.

At the second stage the motion of the particle along the Z axis under gravity is calculated. For this purpose, the maximum distance which can be covered by the particle for one step along the Z axis depending on its mass and magnitude of the time step is split up into portions in proportion to the distance to the nearest particle located not higher than the particle considered. Next, discrete displacement of the particle downwards along the Z axis is considered. The amount of displacement for one step is determined by the indicated splitting. At each step the collision with neighboring particles separately along the X and Y axis is evaluated. Proceeding on this basis, for each axis we determine the direction (opposite to that over which the collision occurred) and the amount of displacement (equal to the magnitude of the collision) that allow the particle considered to bypass the particle with which there was collision. They depend on the arrangement of neighboring particles and on the walls mounted. Several versions of bypassing are possible for the particle: the displacement either along the two axes or along one of

Institute of Engineering Chemistry, Ural Branch, Russian Academy of Sciences, Perm. Translated from Inzhenerno-Fizicheski Zhurnal, Vol. 63, No. 1, pp. 69-71, July, 1992. Original article submitted July 24, 1991.

1062-0125/92/6301-0705$12.50

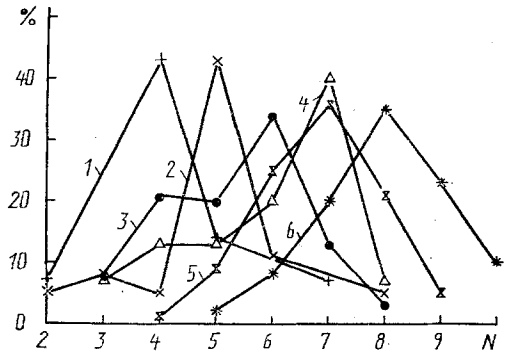

Fig. 1. Distributions of coordination numbers N at different packing porosities P: predicted data: 1) P = 0.50; 2) 0.49; 3) 0.48; 4) 0.45; experimental data [4]: 5) P = 0.45; 6) 0.43.

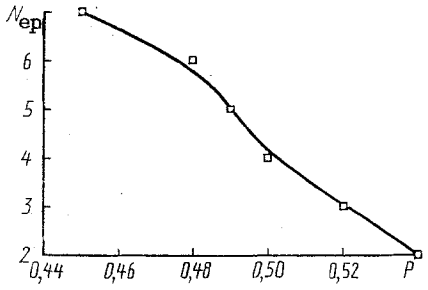

Fig. 2. Mean coordination number N_{ep} vs packing porosity P.

them. In the first instance the particle also displaces along one of the axes, which is found with the help of random choice. And if the neighbouring particles or walls prevent the particle from being displaced in this way, it secures on the previous level. In the case of a positive result (there was no collision or it was prevented), the particle is fixed on the current level. As a consequence of the step-by-step motion the particle settles itself on the minimum possible level. Thereafter, we go over to calculation of the motion of the next particle. The particles having no possibility to move downwards in the volume considered (for example, those lying on the bottom) are subjected only to the effect of vibration. In our opinion, the proposed algorithm allows one to completely exclude running of particles into one another and to obtain a real configuration of particles in space.

As the basic output characteristic, the coordination numbers of all the particles of the packing are calculated. Two particles are assumed to be contacting if the distance between them is not over one tenth of the radius.

The model has been realized as a TURBOPASCAL program written for an IBM PC computer. As a result of a number of calculations, the distributions of the coordination numbers of particles corresponding to different system porosities have been obtained (Fig. 1). By the use of these distributions it is possible to find the dependence of the mean coordination number of particles on porosity (Fig. 2). The results were compared with the experimental data of W. O. Smith [4] obtained as long ago as 1929. The results in the present work were obtained for statistical packings of lead shot. The number of small shot came to 1200-2400. To fix contacting points, the lead was poured with acetic acid as a consequence of which white spots were observed at the places of contact. From the data given in Fig. 2 follows that the proposed model actually reflects statistical packings of spherical particles and allows one to obtain porosity-dependent distributions of coordination numbers also for polyfractional dispersions.

NOTATION

Here h is the initial distance between particles; r, particle radius; φ, volumetric filling of system; φ_m, maximum volumetric filling of system.

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MODEL OF SUSPENSION FILTRATION WITH ACCOUNT OF COLMATATION AND SUFFOSION

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UDC 532.546

A model of suspension filtration is suggested, which takes into account the effects of colmatation and suffosion in a porous medium.

Filtration of suspensions in a porous medium forms the basis for many technical, industrial, and other processes. Among them special attention is given to hydrological (filtration of waters through dams, grounds, etc.) [1], chemical and food [2, 3] processes, as well as to processes of extraction of petroleum and gas [4].

The construction of rather general mathematical models, describing important features typical of the suspension filtration process is the field of investigation, which has been studied until now with insufficient completeness. The results of the separate theoretical and experimental researches are presented in [5-7]. In work [5] a system of equations is derived for determination of the concentration of solid suspensions in liquid n and the saturation density of the porous medium by deposit ρ. The processes of colmatation and suffosion and also the result of their simultaneous action are considered separately in [6]. Together with a balance equation use is made of the equation characterizing the intensity of a change in the deposited mass volume ζ, which is analogous to the equation of the gas adsorption kinetics [8, 9] in the case of a linear dependence of the equilibrium concentration on the concentration of a substance under sorption. Consequently, the equilibrium concentration, at which the process intensity will be equal to zero, depends only on the deposited mass volume. However, as is shown in [10], the intensity of the change of characteristics (in the work we consider the current value of the active porosity but not the volume of the deposited mass) depends not only on the values of n and ε, but on grad p; this fact is confirmed by experimental investigations. In [10] we considered a new model of the filtration, where colmatation and suffosion were taken into account in terms of certain probability coefficients, characterizing the intensity of the blockage and freeing process of pores by fluid particles. However, in [10] we studied the model with concentrated parameters, and the particle distribution in longitudinal and lateral flow directions was disregarded. In this work the model [10] is generalized to the model with distributed parameters.

Suppose that a suspension with the initial volume concentration of solid particles n_0 enters the porous medium filled with a liquid without particles. Because of deposition of the suspension particles, the pores of the medium are blocked, the liquid flow in them is stopped up, i.e. they are disconnected from the filtration process. This fact, naturally, leads to the change in the active porosity. Later the colmated pores may become free of particles under the action of the pressure drop. As in [10], we assume that each deposited particle blocks up one isolated pore and, consequently, changes the active porosity. Then we may write the substance balance equation in the volume unit of the porous medium without reference to convective dispersion in a one-dimensional case as follows

$$\frac{\partial n}{\partial t} + \frac{v(t)}{\varepsilon}\frac{\partial n}{\partial x} = \frac{1}{\varepsilon_0}\frac{\partial \varepsilon}{\partial t}. \qquad (1)$$

M. Ulugbek State Institute for Architecture and Construction, Samarkand. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 63, No. 1, pp. 72-79, July, 1992. Original article submitted February 7, 1991.

1062-0125/92/6301-0707$12.50