Journal of Engineering Physics and Thermophysics, Vol. 74, No. 5, 2001

CHAOTIC HOMOGENEOUS POROUS MEDIA. 1. STRUCTURE THEOREMS

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UDC 536.24:544.77

Basic theorems of the structure of the chaotic homogeneous isotropic porous media that form the first group of theorems of transport theory in disordered systems are presented in the work.

The theory of heat exchange in stochastic porous systems presupposes the development of probability-theoretic analysis of four principal interrelated trends: a structural theory, conservation laws, hydrodynamics, and heat exchange [1]. The present work is devoted to the first part of the analysis, i.e., to the elementary structural theory.

Definition. If, for any cross section of a chaotic porous medium, the probability distribution of porosity (clearance) over the area is single and unimodal, this medium is called *homogeneous and isotropic*.

Theorem 1. *For a homogeneous and isotropic chaotic porous medium, the mean porosity over any cross section is equal to the volume porosity* $\overline{\Pi}_S = \overline{\Pi}_V = \overline{\Pi}$. The proof follows from ergodicity (see Theorem 7) and the well-known analysis theorem $V_{[a,b]} = \int_a^b S(x)dx$.

Chaotic Spherical Packings (Charges) d_{part} = const. **Theorem 2.** *In chaotic spherical packings with a large number of particles:*

(1) *the porosity* is $\overline{\Pi}_S = \overline{\Pi}_V = \overline{\Pi}$;

(2) *the specific wetted perimeter* is $\overline{P} = \dfrac{3\pi(1-\overline{\Pi})}{2d_{\text{part}}}$;

(3) *the hydraulic diameter* is $d_{\text{hyd}} = \dfrac{4\overline{F}}{\overline{P}} = \dfrac{8}{3\pi}\dfrac{\overline{\Pi}}{(1-\overline{\Pi})}d_{\text{part}}$.

Proof. If the mean volume porosity is $\overline{\Pi}_V$, the mean volume concentration of particles is $\overline{n}_V = 6(1-\overline{\Pi}_V)/(\pi d_{\text{part}}^3)$. Then the number of particles completely or partially located in a plane layer of thickness d_{part} can be characterized by the mean surface concentration $\overline{n}_S = \overline{n}_V d_{\text{part}}$.

We bring the cross-sectional plane into coincidence with the plane *XOY* (Fig. 1) and consider the distribution of the coordinates of the centers of spheres occurring in the plane layer $-r_{\text{part}} \le z \le r_{\text{part}}$, $-\infty < x < \infty$, and $-\infty < y < \infty$. From the population of all the spheres completely or partially entering into the layer, we perform a random sampling of spheres, the distance between which exceeds the correlation radius R_{cor} (the short-range order). For the coordinate *Z* of the centers of the spheres of such samples, a uniform distribution (isotropy in the large) holds true. But the entire population can be covered by the counting number of such samples. Therefore, the total probability density is $f(z) = 1/d_{\text{part}}$. From this, for the mean cross-sectional area $\overline{s}_0$, the specific cross section of particles on the plane $\overline{s}_S$, the mean cross-sectional perimeter $\overline{P}_0$, the specific perimeter $\overline{P}$, the hydraulic diameter d_{hyd}, and the equivalent diameter d_{eq} we obtain

"Algorithm-M" Joint-Stock Association, Moscow, Russia; email: mog_@mail.ru. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 74, No. 5, pp. 196–200, September–October, 2001. Original article submitted May 23, 2000; revision submitted May 8, 2001.

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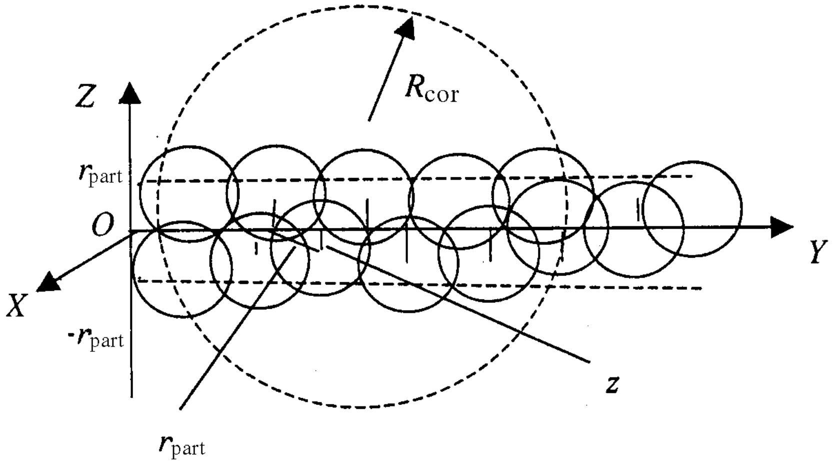

Fig. 1. Section of the chaotic packing by the plane.

TABLE 1. Basic Ordered Packings of Spheres

Type of packing	Coordination number	$1-\Pi$	Π
Most dense packing	12	$\frac{\sqrt{2}}{6}\pi = 0.7405$	0.2595
Cubic packing	6	$\frac{\pi}{6} = 0.5236$	0.4764
Tetrahedral packing	4	$\frac{\sqrt{3}\pi}{16} = 0.3401$	0.6599
Least dense packing (unstable equilibrium)	4	$\frac{2\sqrt{3}\pi}{(\sqrt{6}+2)^3} = 0.1235$	0.8765

$$\bar{s}_0 = \frac{\pi d_{part}^2}{6}, \quad \bar{s}_S = \bar{s}_0 \bar{n}_S = 1 - \overline{\Pi}_V; \quad \overline{\Pi}_S = 1 - \bar{s}_S = 1 - (1 - \overline{\Pi}_V) = \overline{\Pi}_V,$$

$$\overline{P}_0 = \frac{\pi^2 d_{part}}{4}, \quad \overline{P} = \overline{P}_0 \bar{n}_S = \frac{3\pi (1 - \overline{\Pi})}{2 d_{part}}, \quad d_{hyd} = \frac{4\overline{F}}{\overline{P}} = \frac{4\overline{\Pi}}{\overline{P}} = \frac{8}{3\pi} \frac{\overline{\Pi}}{1 - \overline{\Pi}} d_{part},$$

$$d_{eq} = \frac{2}{3} \frac{\overline{\Pi}}{1 - \overline{\Pi}}; \quad \frac{d_{hyd}}{d_{eq}} = \frac{4}{\pi} \approx 1.27.$$

Hereafter, the values of the porosity of certain ordered packings will be used (see Table 1) [2].

Theorem 3. (Yu. A. Buevich, (1968) [3]). *In chaotic dense spherical packings with a large number of particles, the volume distribution of the particles obeys the normal law*

$$W(n) = [2\pi N_V \nu (1-\nu)]^{-1/2} \exp\left[-\frac{(n - \nu N_V)^2}{2 N_V \nu (1-\nu)}\right].$$

Here $W(n)$ is the probability density of occurrence of n particles in N_V cells of volume V; $N = (1 - \Pi_{min})V/V_{part}$; ν is the fraction of cells occupied by the particles $\nu = (1 - \Pi)/(1 - \Pi_{min})$; N, $n \gg 1$.

The proof is based on the scheme of random unrepeated sampling in a discrete lattice space with the use of the De Moivre–Laplace limiting theorem.

Corollary 1. The volume porosity distribution obeys the normal law. Since $\Pi = 1 - \frac{nV_{\text{part}}}{V}$, we have

$$W(\Pi) = \frac{1}{\sigma_1 \sqrt{2\pi}} \exp\left[-\frac{(\Pi - \overline{\Pi})^2}{2\sigma_1^2}\right], \quad \sigma_1^2 = \frac{(1 - \overline{\Pi})(\overline{\Pi} - \Pi_{\min})V_{\text{part}}}{(1 - \Pi_{\min})V}.$$

Corollary 2. A spherical packing with a large number of particles is a volume containing more than 3000 elements. The hypergeometric distribution goes over asymptotically into a normal distribution with the total number of particles [4, 5]

$$N_{\text{part}} > \frac{90}{\nu(1-\nu)^2};$$

therefore, for $\overline{\Pi} = 0.4$ and $\Pi_{\min} = 0.26$ we obtain $N_{\text{part}} > 3000$.

Theorem 4. *Chaotic spherical packings are homogeneous and isotropic porous media.*

Proof. Since $\Pi_S = 1 - \frac{\bar{s}_0 n}{S}$, where $\bar{s}_0 = \frac{\Pi d_{\text{part}}^2}{6}$ and n is the random number of particles in the plane layer $V = Sd_{\text{part}}$, we have

$$W(\Pi_S) = \frac{1}{\sigma_2 \sqrt{2\pi}} \exp\left[-\frac{(\Pi_S - \overline{\Pi})^2}{2\sigma_2^2}\right], \quad \sigma_2^2 = \frac{(1 - \overline{\Pi})(\overline{\Pi} - \Pi_{\min})\bar{s}_0}{(1 - \Pi_{\min})S}.$$

Theorem 5. *If* $\Pi_{\min} \le \Pi \le \Pi_{\max}$, *then*

$$W(\Pi) = \frac{1}{\sigma_3 \sqrt{2\pi}} \exp\left[-\frac{(\Pi - \overline{\Pi})^2}{2\sigma_3^2}\right]. \quad (1)$$

Here

$$\sigma_3^2 = \frac{(\Pi_{\max} - \overline{\Pi})(\overline{\Pi} - \Pi_{\min})}{(\Pi_{\max} - \Pi_{\min})} K; \quad K = \begin{cases} \dfrac{V_{\text{part}}}{V} & \text{– for volume,} \\ \dfrac{\bar{s}_0}{S} & \text{– for area.} \end{cases}$$

The proof is similar to that of Theorems 3 and 4.

Mean Porosity of the Chaotic Spherical Charge. The experimental data of [6–9]: $\overline{\Pi} = 0.38$–0.41 is the spherical charge without additional mechanical actions; $\overline{\Pi} = 0.35$–0.39 is the spherical charge with subsequent vibration or shaking; Scott [7] investigated the filling of spherical vessels of different dimensions with spheres: $\overline{\Pi} = 0.40 + 0.37/N_{\text{part}}^{1/3}$ (without vibration) and $\overline{\Pi} = 0.36 + 0.33/N_{\text{part}}^{1/3}$ (with simultaneous shaking).

Physical assumptions: (1) $\Pi_{\min} = 0.26$ corresponds to the most dense packing (hexagonal, face-centered cubic, and certain not lattice structures; coordination number 12); (2) granular media that occur in a gravitational field and are subjected to mixing, vibration, and other additional mechanical actions cannot be very loose, i.e., for example, unstable configurations in the charge with $\Pi_{\max} = 0.791$ (coordination number 4) are excluded. It can be assumed that the least dense granular medium under these conditions is characterized by the porosity of a regular cubic packing with coordination number 6 and $\Pi_{\max} = 0.476$. Indeed, in the case of a regular cubic arrangement the mechanical actions cause the spherical particles to shift from the initial positions and the density of the medium to increase. On the other hand, the legitimacy of the second assumption made is confirmed by the results of investigations in the region of phase transitions. It is well known that the stability limit of systems of irregularly arranged molecules is attained for a density corresponding to that of a cubic packing.

Theorem 6. *In an infinite chaotic spherical charge, produced as a result of mechanical action (mixing, vibration, etc.) in a gravity field, the entropy maximum of the probability distribution of the porosity is attained for* $\Pi = 0.37$.

Proof. The entropy of the probability distribution for the random porosity is

$$H = -\int_{-\infty}^{+\infty} W(\Pi) \ln W(\Pi)\, d\Pi .$$

For a spherical charge we have

$$H = \frac{1}{2} \ln 2\pi e \sigma_3^2 .$$

Whence

$$H_{max} = \frac{1}{2} \ln \frac{\pi e K}{2} (\Pi_{max} - \Pi_{min}) \quad \text{for} \quad \overline{\Pi} = \frac{\Pi_{min} + \Pi_{max}}{2} = 0.37 .$$

Corollary. In densely filling a limited volume, the mean porosity of the charge is $\overline{\Pi} = 0.37 + k/N^{1/3}$, where k is the coefficient dependent on the shape of the filled vessel. The particles located near the vessel walls are in a particular position compared to the particles in the volume and affect the packing density. The magnitude of their contribution is proportional to the ratio of the surface area R^2 to the vessel volume R^3, i.e., the porosity of the charge increases in inverse proportion to the dimension of the system R or $N^{1/3}$, since the system volume is in proportion to the total number of spheres. In experiments with spherical vessels, the numerical coefficient is $k = 0.33$ with vibration and $k = 0.37$ without vibration.

When the mechanical action is absent, Π_{max} and $\overline{\Pi}$ increase insignificantly due to the existence of less dense unstable configuration inclusions than cubic ones.

We note that a similar result leading to the entropy maximum for $\overline{\Pi} = (\Pi_{min} + \Pi_{max})/2$ also holds true for a discrete binomial distribution, from which a limited normal distribution is obtained in Theorem 3.

Basic Theorem of the Structure of Homogeneous Isotropic Porous Media. Theorem 7. *A chaotic medium is homogeneous and isotropic if and only if at any cross section the probability distribution of porosity over the area obeys the normal law*

$$W(\Pi) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{(\Pi - \overline{\Pi})^2}{2\sigma^2}\right], \quad \sigma^2 = D[\Pi] = \overline{\Pi}(1 - \overline{\Pi})\left(\frac{d_D}{d_S}\right)^2 . \tag{2}$$

Here d_D is the dispersion diameter, which is the basic linear characteristic of the porous homogeneous structure and d_S is the diameter of the arbitrary circular region of the cross section $S = \pi d_S^2/4$.

The sufficiency is obvious; it follows from the definition of a homogeneous isotropic porous medium.

To prove the necessity, we use a diagram of the Monte Carlo method (Fig. 2). Let N_0 random uniformly distributed points be arbitrarily selected on the cross-sectional area S_0. Part of the points $N_{0,\Pi}$ are located in pores; the mean porosity $\overline{\Pi}$ is determined in an ordinary manner ($\overline{\Pi} = S_{0,\Pi}/S_0$, where $S_{0,\Pi}$ is the

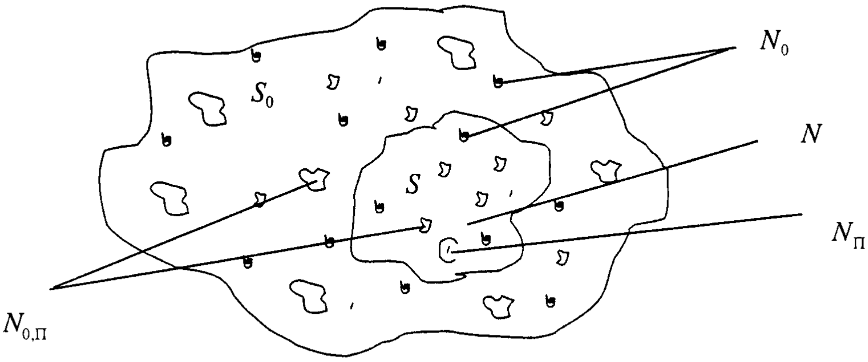

Fig. 2. Proof of the basic theorem.

area of the pores in the cross section). Then for the random quantity $N_{0,\Pi}/N_0$ the relation $\frac{N_{0,\Pi}}{N_0} = \frac{1}{N_0}\sum_{i=1}^{N_0}\xi_i$ with a uniform distribution for $\xi = \begin{pmatrix} 1 & 0 \\ \overline{\Pi} & 1-\overline{\Pi} \end{pmatrix}$ holds true. The quantity $N_{0,\Pi}/N_0$ for $N_0 \to \infty$ is asymptotically normal with mathematical expectation $M\left[\frac{N_{0,\Pi}}{N_0}\right] = \overline{\Pi}$ and dispersion $D\left[\frac{N_{0,\Pi}}{N}\right] = \frac{\overline{\Pi}(1-\overline{\Pi})}{N_0}$. Then, for example, according to the "rule of three-sigmas" we obtain

$$P\left(\left|\frac{N_{0,\Pi}}{N_0} - \overline{\Pi}\right| < \frac{3\sqrt{\overline{\Pi}\,(1-\overline{\Pi})}}{\sqrt{N_0}}\right) = 0.997\,.$$

The last relation justifies the use of the Monte Carlo method for determining the mean porosity for $N_0 >> 1$. We select the region with area S in the cross section; $S < S_0$; N is the total number of random points; N_Π is the number of random points in the pores; $\Pi = S_\Pi/S$ is the porosity of the region S. Then it is easy to show that, first:

$$P\left(\left|\frac{N}{N_0} - \frac{S}{S_0}\right| < \frac{\sqrt[3]{\left(\frac{S}{S_0}\left(1-\frac{S}{S_0}\right)\right)}}{\sqrt{N_0}}\right) = 0.997$$

and, second, by means of the unrepeated-sampling model:

$$W(N_\Pi) = \frac{C_{N_{0,\Pi}}^{N_\Pi}\, C_{N_0 - N_{0,\Pi}}^{N-N_\Pi}}{C_{N_0}^{N}}\,.$$

For $N/N_0 << 1$, $N/N_{0,\Pi} << 1$, and $N/(N_0 - N_{0,\Pi}) << 1$, using the de Moivre–Laplace limiting theorem and considering that $N_\Pi/N = \Pi$ for N_Π and $N >> 1$, we have

$$W(\Pi) = [2\pi\overline{\Pi}\,(1-\overline{\Pi})/N]^{-1/2} \exp\left[-\frac{N\,(\Pi-\overline{\Pi})^2}{2\overline{\Pi}\,(1-\overline{\Pi})}\right].$$

Here $N/N_0 = S/S_0$ or $N_0/S_0 = N/S = 1/S_D$ for any area S; similarly it is easy to show that $N_0/S_0 = N_\Pi/S_\Pi = 1/S_D$ for the corresponding area of the pores S_Π; therefore, S_D is independent of the area and porosity and is the characteristic of the structure. For $S_D = \pi d_D^2/4$, we finally obtain the normal law (2). The theorem is proved.

Corollary 1. For chaotic homogeneous isotropic porous media, the probability distribution of the porosity over the volume obeys the normal law. The proof is similar.

Corollary 2. Of all the continuous distributions the normal distribution has the greatest entropy for the given dispersion. This well-known result of variational calculus is the thermodynamic substantiation and confirmation of the prevalence of homogeneous isotropic porous systems in nature and of the normal law of porosity distribution in these systems.

Corollary 3. The dispersion diameter for a spherical charge is determined by the formula

$$d_D = \frac{\sigma d_S}{\sqrt{\overline{\Pi}\,(1-\overline{\Pi})}} = \left[\frac{2\,(\Pi_{\max}-\overline{\Pi})\,(\overline{\Pi}-\Pi_{\min})}{3\,(\Pi_{\max}-\Pi_{\min})\,(1-\overline{\Pi})\,\overline{\Pi}}\right]^{1/2} d_{\text{part}}\,, \tag{3}$$

which follows from relations (1) and (2). For $\overline{\Pi} = 0.37$, $\Pi_{\min} = 0.26$, and $\Pi_{\max} = 0.476$ we obtain $d_{\text{hyd}} = 0.499 d_{\text{part}} \approx 0.5 d_{\text{part}}$, $d_{\text{eq}} = 0.392 d_{\text{part}} \approx 0.39 d_{\text{part}}$, and $d_D = 0.394 d_{\text{part}} \approx 0.39 d_{\text{part}}$. In this case, the equivalent diameter is almost equal to the dispersion diameter, $d_{\text{eq}} \approx d_D$, which is an important factor in using the experimental data where d_{eq} is the determining dimension.

Corollary 4. The mean value of the porosity over the ensemble $\langle\Pi\rangle$ is equal to that of the porosity over the area (volume) $\overline{\Pi}$, since $\langle\Pi\rangle = M[\Pi] = \overline{\Pi}$. The ergodic property of the mean values of the porosity is proved.

Chaotic deviations of the true porosity of a body from the mean porosity cause the appearance of local dispersion flows. The characteristic scales of this stationary turbulence coincide with the scales of inhomogeneity of a porous body and determine mainly the processes of heat and mass exchange in it, which has been shown by theoretical and experimental investigations [10–16].

NOTATION

Π, porosity; V, volume; S, area; S_D, dispersion area; d_{part} and r_{part}, diameter and radius of the particles; d_{hyd}, d_{eq}, and d_D, hydraulic, equivalent, and dispersion diameters; P, perimeter; F, flow area; n_V and n_S, concentration of particles by volume and area; R_{cor}, correlation radius; s_0, cross-sectional area of a particle; $\overline{s}_S$, specific cross section of the particles; P_0, perimeter of the particle cross section; W, probability density; n, number of particles in the volume V; N_V, number of cells of the volume V; N_{part}, total number of particles; ν, fraction of the cells occupied by the particles; σ, σ_1, σ_2, and σ_3, standard deviations; R, linear dimension of the spherical packing; D, dispersion; N_0, $N_{0,\Pi}$, N, and N_Π, number of random points on the area S_0, $S_{0,\Pi}$, S, and S_Π; ξ, uniformly distributed random quantity; M, mathematical expectation. Subscripts: V, relating to the volume; S, relating to the area; max and min, maximum and minimum values.

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