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MATHEMATICAL SIMULATION OF THE STRUCTURAL PROPERTIES OF PACKED AND FLUIDIZED BEDS

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Based on the algorithm of successive filling a given volume with single spheres, a mathematical model of random packing of a limited volume of a bed in the field of body forces has been developed. This model can be applied to electrothermal packed- and fluidized-bed furnaces and will make it possible to investigate the thermal and electrical conductivity of such beds. A check of the adequacy of the model showed its correspondence to the well-known experimental and calculated results, as well as the stability of the solutions obtained with its aid.

Keywords: *random packing of particles, bed conductivity, packing density, voidage, coordination number, elementary volume, near-wall zone.*

Introduction. Heat and mass transfer in bed apparatuses is determined in many respects by the properties of the granular structure of a bed and by the granulometric composition of the material, as well as by the packing density and coordination number. The influence of the packing is especially appreciable in electrothermal dense- and fluidized-bed furnaces in which the intensity and distribution of the Joule heat sources are directly determined by the conditions of the contact interaction of elements [1–5].

The processes associated with high-temperature processing of a carbon-containing material in electrothermal furnaces have a complex physical character. The most probable mechanisms underlying the release of heat are the electrocontact and electrospark heating in the bulk of the bed as a result of the interaction of bed particles with one another. To estimate the electrical conductivity of granular structures, the approach of [6] can be used that accounts for the size and roughness of particles, number of contacts, and the mechanical load:

$$\Lambda = \frac{G}{G_0} = \left(\frac{y_1}{y_4}\right)^2 \left(0.5\overline{h}_r + \left(1 - 0.5\overline{h}_r\right)\Phi\right)^{-1}, \tag{1}$$

$$y_4 = \frac{2\sqrt{N-1}/N}{\sqrt[3]{1-\varepsilon}}, \tag{2}$$

$$\Phi \approx 0.017 + 0.4 y_1, \tag{3}$$

$$\overline{h}_r = \frac{h_r}{d/2}, \tag{4}$$

$$y_1 = K\sqrt{\eta}\sqrt[3]{(1-\varepsilon)^{-2/3} P}, \tag{5}$$

where $\eta = (0.001–1)\cdot 10^{-2}$ is the relative area of an actual contact depending on the shape and size of the microroughness, strength characteristics, and on the magnitude of outer load. The use of Eqs. (1)–(5) presupposes knowledge of the structural properties of granular systems: voidage and coordination number. One of the main methods of studying these systems is simulation. The practical implementation of such mathematical models allows one to pass to considering structures with specific geometric parameters. In this case, the elements (grains) themselves with known coordinates form a kind of a skeleton where each connection line corresponds to one unique contact.

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Thus, the solution of the geometric problem of identifying the skeleton structure of a bed together with simulation of the conductivity of the individual contacts [4] and of the skeleton as a whole allows one to investigate the processes of heat and mass transfer in electrothermal packed- and fluidized-bed furnaces. The present work is aimed at simulating the geometric characteristic features of the packing of a granular bed structure in the context of studying the bed conductivity.

The solutions of the problems of close packing of particles have found a wide application in science and technology. Such solutions are used for studying the contact conductivity of granular systems [6]; in modeling the molecular and atomic structure of a substance [7, 8]; in nanotechnologies [9] and the theory of information coding [10]; in optimizing the space occupation [11]; in studying the properties of grounds [12], filtering charges and powder materials [13–15], as well as the processes of physical adsorption [16] and filtration combustion [17]. Interest in the indicated problems has increased considerably in recent years in view of the development of the modern means of modeling and visualization [18–38].

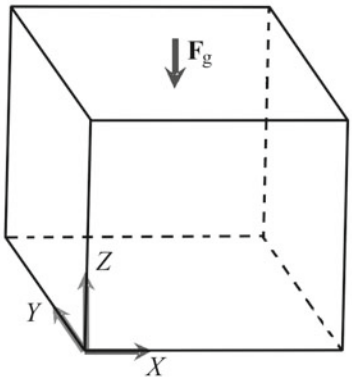
An analysis of works [6–38] shows that despite the commonness of the problems listed above, each individual case has its own specific features that determine the validity of one or another assumption. For example, it is advisable to consider the packing of a bed in an industrial furnace as a random charge of a material and to calculate it with account for the acting body forces (gravitation and inertia), the inhomogeneity of the granulometric composition, shape of the material, and for the limited volume of the working space. This brings up a number of accompanying questions about the dimensions of the elementary volume that has the characteristics of the bed core, the dimensions and influence of the near-wall region, density fluctuation, and about the coordination number of packing.

The reported results of experimental and theoretical investigations of structural properties of packings are ambiguous [13, 15, 18, 21, 24–30, 37]. Most of the results lead to the conclusion that the density of a random packing φ ranges from 0.54 to 0.65. As to the coordination number N, there is no uniformity of opinion. In the works of R. I. Ayukaev, V. A. Kivran, and I. É. Naats [26–28], from the results of the mathematical simulation of a charge of monodisperse spheres the expected value of the coordination number was determined to be $N = 8$ by the method of successive filling of a volume. On going to a two-component mixture with the ratio of the diameters of spheres 1:2, this index approaches $N = 11$. Analogous results were obtained by T. P. Bondareva for single spheres in [21]. However, the latter author used an algorithm of layer-by-layer filling of the volume without account for the influence of its boundaries, with the coordination number being found from the generalized exponential distribution law. In the work of Sai S. Tulluri [35], the maximum of the probability density of the coordination number obtained for a random packing of spheres by the Monte Carlo method amounted to $N = 6.7$. The results given in [21, 25–28] agree well with the experiments in which the free space in the bed was filled with acetic acid and paraffin to mark the contacts [38]. At the same time, despite the correlation between experimental and calculated data, notion should be made of the discrepancy between them for the probability of the distribution of the coordination numbers. The experimental values for the coordination numbers of identical spheres differ substantially from the theoretical values: $N = 5.9 \pm 0.3$ obtained by Z. Yaremko [24]. As a model liquid in the experiments in [24] a solution of gelatin was used. It is interesting that in the vicinity of each sphere of diameter d there were on the average 10.8 ± 0.6 neighbors at a distance of the order of $0.05d$.

With allowance for the foregoing, attention should be paid to the conclusion drawn by some researchers on the relationship between the structure of random packing and the algorithm of the formation of this packing [18, 24], which may provide an explanation for the disagreement between experimental and predicted data. Analyzing the function $N(\varphi)$ for regular face-centered, body-centered, simple cubic, and diamond packings ($N = 12, 8, 6, 4$), M. N. Magomedov isolated a region of uncertain values of φ corresponding, in his opinion, to random systems [18]. As a result, he suggested an interval characteristic for a random atomic structure of a substance: $N = 5.84–6.32$, $\varphi = 0.454–0.573$. However, in all probability, this estimate cannot be extended to the granular structures of furnaces, since at $N = 4–5$ the bed is not stable [14]. At the same time, the conclusions made by the authors in [18] are confirmed by a number of theoretical works [29, 30, 37, 38].

Thus, the results of investigations of the structural properties of a granular bed need refinement. The aim of the present work is to develop a mathematical model of a random packing of particles of a material of homogeneous fractional composition under conditions of the acting directed body force and to determine the main characteristics of the bed: packing density, coordination number, dimensions of the elementary volume, and of the near-wall region.

Techniques. As the basic method of simulation we used the algorithm of successive filling of a cubic volume (scene) [21, 23, 27, 37] of size $1 \times 1 \times 1$ by single spheres of different diameters (Fig. 1). The forces of mechanical interaction were not taken into account, and the problem of finding a stable position of a sphere in a dimple was reduced to the search for optimum coordinates of its center at which a shift in the direction of the gravity vector $\mathbf{F}_g$ becomes impossible ($\Delta n \to 0$). The criterion of the optimum solution is the fulfillment of the following conditions:



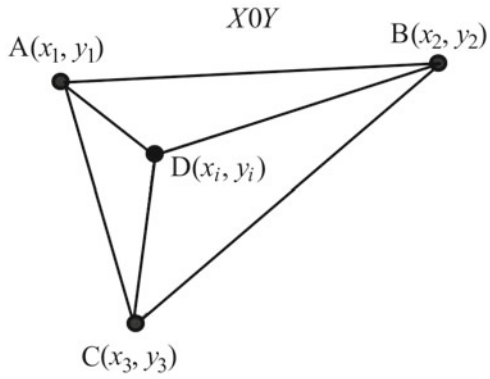


Fig. 1. Region of filling with granular packing.

Fig. 2. Condition of equilibrium position of a sphere in a dimple: A, B, C, D, projections of supporting contacts and of the sphere center of mass onto the $X0Y$ plane.

residence of the ith sphere within the scene

$$r_i \le x_i \le 1 - r_i \,, \quad r_i \le y_i \le 1 - r_i \,, \quad z_i \ge r_i \,, \tag{6}$$

nonintersection of spheres

$$(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 \ge (r_i + r_j)^2 \,, \tag{7}$$

the presence of no fewer than three supporting contacts, each of which satisfies one of the equalities

$$(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 \ge (r_i + r_j)^2 \,,$$

$$x_i = r_i \cup x_i = 1 - r_i \,, \quad y_i = r_i \cup y_i = 1 - r_i \,. \tag{8}$$

The equilibrium position of a sphere in a dimple is determined by the equality of the acting gravity forces and reactions of the support $\Sigma\mathbf{F} = 0$ [37, 40]. Therefore, it is essential that the vector of the gravity forces from the center of mass of the sphere be able get into the triangle of area S_{ABD}, S_{BCD} or S_{ACD} formed by the projection of three supporting contacts onto the $X0Y$ plane (Fig. 2). In a numerical experiment, in the course of filling the volume, the initial coordinates x and y beyond the scene ($z > 1$) were given for each new sphere in a random way, as well as the diameter according to the initial granulometric composition. After this, the sphere was lowered with the step $\Delta n = r/4$ down to the bed surface. Further search for the dimple was made by the Monte Carlo method and involved investigation of the given vicinity of radius r by successive subdivision of the step Δn with account for the limitations (6) and (7). At $\Delta n = 0$ the presence of the supporting contacts (8) was checked as well as the fulfillment of the equilibrium condition (Fig. 2). The spheres were considered contacting at the distance between their centers equal to $\Delta = r_i + r_j$ with an error $\delta \le 1\%$. In the case of a negative result of the checking, the value of the step $\Delta n = r/4$ was recovered for the current position of the sphere.

The given algorithm was realized in the Visual Basic language. The relative mean diameter of spheres d was taken equal to 0.025. This corresponds to successive deployment of up to 40 rows of elements along the wall, thus minimizing the influence of the near-wall effects in the formation of the bed core structure [13, 28, 33, 39]. The number of spheres was of the order of 64 thousand. The packings were visualized by the AutoCAD and CadTools means (Fig. 3).

Results of Discussion. As a result of 20 numerical experiments the conclusion was drawn that for a disordered bed of 64 thousand of identical spheres formed in the field of the acting body force in a limited volume, the voidage ε is equal to 0.406–0.408 ($\varphi = 0.592$–0.594) and the coordination number is $N = 6.11$–6.14. As is seen, the mathematical model satisfies the convergence and stability criteria of solutions. It should be noted that with higher demands on the error of packing ($\delta \le 0.1\%$), the value of ε asymptotically approaches 0.4, with the average value of N remaining the same. Visual inspection of individual fragments of the bed (Fig. 3) has revealed no discrepancy with the described algorithm and with the used restrictions. Thus, the results obtained agree to the greatest extent with the experimental and calculated data of works [18, 24, 25].

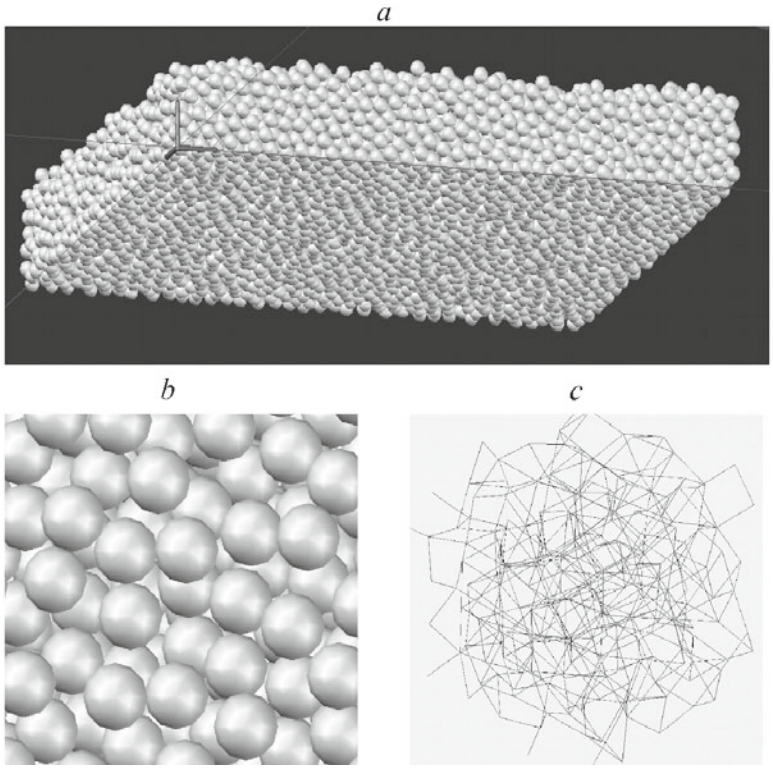


Fig. 3. Visualization of a disordered bed of identical-diameter spheres in the field of directed body force: a) a fragment of a bed of 10 thousand spheres; b) a fragment of the bed surface; c) skeleton of the bed core (6 × 6 × 6)*d*.

An analysis of packings has shown that the distribution of the coordination numbers for the entire array of spheres obeys the normal Gauss law (Fig. 4). The number of contacts takes the values from 3 to 9, with the lower limit of the indicated range corresponding to the spheres located on the bed surface. The probability maximum $f(N) = 0.46$ is observed for the contact number $N = 6$. In individual packings there are spheres with $N = 10$ and 11, but this is rather an exception from the general tendency. According to the results of investigations of the vicinity of spheres at distances of 1.05*d*, 1.1*d*, and 1.25*d*, the number of neighbors came to 6.8, 7.7, and 10.0, respectively. Thus, the coordination number determined in the numerical experiment for a disordered single bed $N = 6.11$–6.14 turned out to be far from the value 8. Moreover, the predicted distance between neighbors (curves 1–3) differ substantially from the expert estimate [24]. The reasons may be both the absence of exact measurements of this index in experiments [24] and some of the assumptions of the model (curves 1–3) that do not account for the specific features of the dynamics and statics in the course of filling: the presence of friction forces, elastic interactions, rolling of spheres, etc.

An important stage in the analysis of the model of the bed is the interpretation of results. For a random packing, use is often made of the so-called radial function of random filling $g(R)$ that in essence is the dependence of the integral density of packing on the radius of a sphere as the center of which a certain base reference point is selected [26]. However, in modeling the conductivity in application to electrothermal furnaces it is convenient to consider rectangular elementary volumes, which facilitates the determination of such parameters as the thermal conductivity coefficient or specific electrical resistance of the bed.

At the first stage we investigated the transparency ε_f of the square sections of the bed at the mark $z = 0.45$ parallel to the $X0Y$ plane. The sizes of the sections varied from 1.5*d* to 20*d*. The transparency was calculated as a fraction of the space free of the material and simultaneously the average number of contacts was determined for spheres in the given section. As is seen from Fig. 5, already at (8–9)*d* the transparency of the bed core coincides with its voidage (curves 1–3). Near the wall regions the values of ε_f differ (curves 4–6), but the general picture of the interconnection remains the same. As to the coordination number, it takes characteristic values of the bed core at the size of the area equal to about 10*d* and the bed boundaries, to about 12*d*.

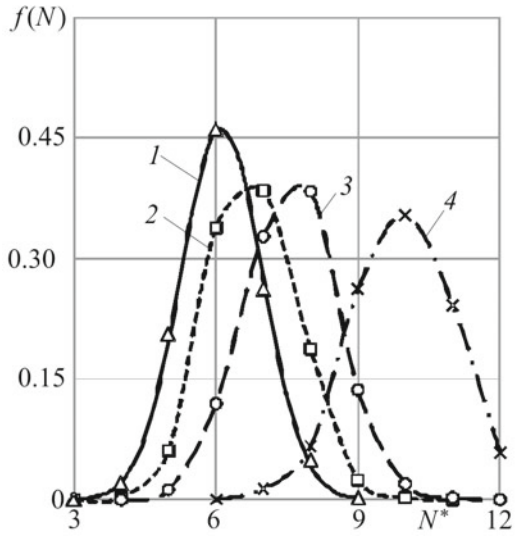


Fig. 4. Probability density of the distribution of neighbors in the vicinity of spheres of radius 1d ($N^* = N$) (1), 1.05d (2), 1.10d (3), and 1.25d (4).

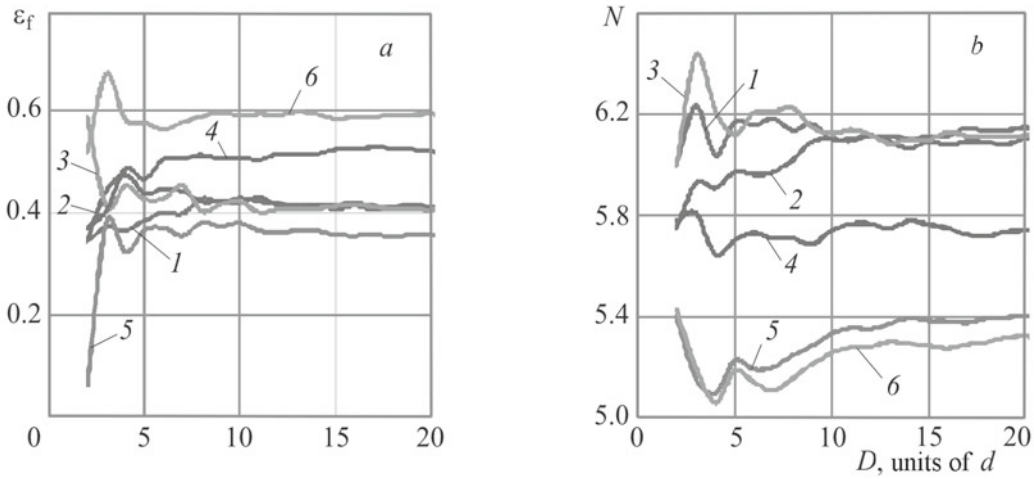


Fig. 5. Transparency of ε_f (a) and coordination number N (b) of a monodisperse bed of spheres depending on the size of the elemental area D: 1) $r = 20d$; 2) $10d$; 3) $5d$; 4) $1d$; 5) $0.5d$; 6) $0.25d$.

Thus, with a certain extent of assumption the elemental area of section $12 \times 12d$ can be considered to be representative of the properties of random packings. This is also confirmed by the changes in the values of ε_f and N when the elemental area $(12 \times 12)d$ moves in the direction of the $0Y$ axis (Fig. 6) from the side wall and deep in the bed. Moreover, the behavior of the function $\varepsilon_f(y)$ in the wall region correlates with the familiar experimental and calculated data of [13, 15, 28]. The fluctuation of the transparency and of the coordination number inside the bed (Fig. 6) are within ±8% and ±2.5%, whereas at a distance of $1.5d$ from the wall the unit area already acquires the characteristics of the core.

The bed is characterized better by such an integral volumetric index as voidage. With passage from the elemental plane square section to a cubical segment (Fig. 7) it is seen that the fragments (cubes) of size more than $(6 \times 6 \times 6)d(216d^3)$ possess all the properties of the core. Taking into account the fact that a plane area of size $(10 \times 10)d$ (Fig. 5, curve 1–3) indirectly characterizes a certain vicinity $\pm d$ in the $0Y$ direction of volume $(10 \times 10 \times 2)d = 200d^3$, a conclusion can be drawn about the coincidences of the results presented in Figs. 5 and 6. Thus, as a unit bed of monodisperse spheres a volume of about $200d^3$ should be used in modeling the conductivity. This conclusion allows one to substantially reduce the boundaries of the region of simulation of the contact conductivity of granular structures.

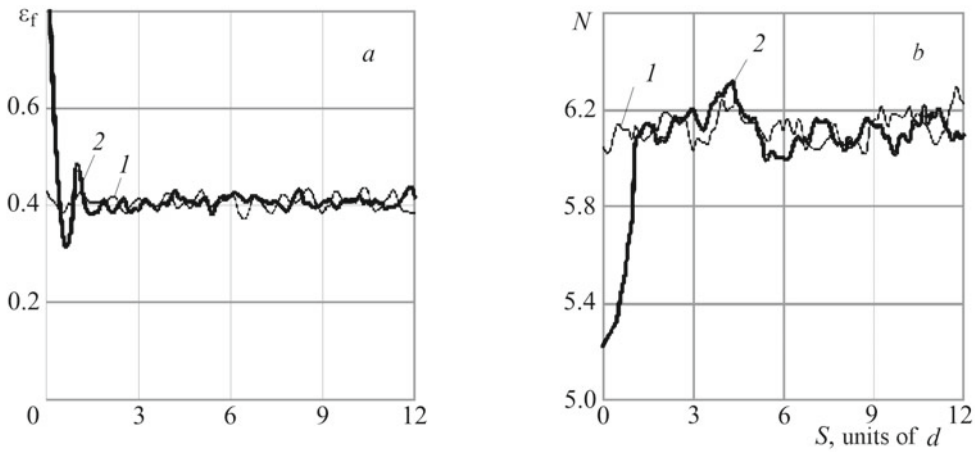


Fig. 6. Fluctuations of transparency of ε_f (a) and of coordination number N (b) of a monodisperse bed of spheres at $D = (12 \times 12)d$; 1) bed core; 2) vicinity of a wall.

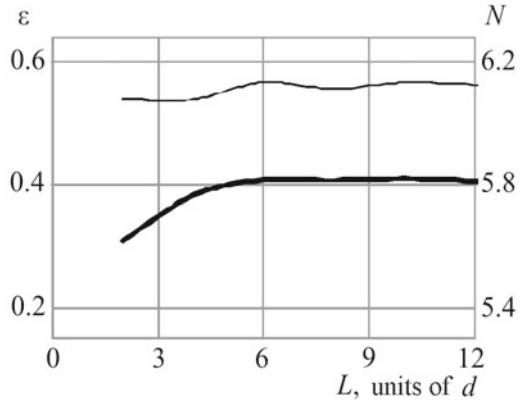


Fig. 7. Voidage ε (1) and coordination number N (2) vs. the linear dimension of an elementary volume.

TABLE 1. Influence of the Diameter of Graphite Particles on the Specific Electrical Resistance of a Bubbling Bed at $t = 20^{o}$C

Particle diameter, mm	Ω, Ω·cm	
	Calculation	Experiment [42]
0.105	34	33
0.195	27	27
0.375	23	24
0.850	21	23

An analysis of the conductivity of an electrothermal bubbling bed was carried out on the basis of a two-phase model [39, 41]. In this case, the system consists of gas bubbles and of a conventionally "dense" emulsion phase that plays the role of the electric energy conductor. Using the data obtained in simulation for the voidage and coordination number, as well as relations (1)–(5), we determined the values of the specific electrical resistance of a bubbling bed of graphite (Table 1) that give satisfactory agreement with experimental data. In such a case, the value of the roughness $h_r = 1.5 \cdot 10^{-3}$ mm and the relative radius of the spot of the actual contact $y_1 = 2.5 \cdot 10^{-3}$ mm are adopted in accordance with the recommendations given in [4].

CONCLUSIONS

1. The characteristics of random packings change in wide ranges: φ = 0.45–0.65 and N = 6–8. The lack of agreement between the experimental and calculated data, well-known from the literature, is due to the differences in the methods of granular structure formation, physical specific features of the pertinent problems, as well as to the subjective factors associated with the errors occurring in measurements and modeling.

2. For a given cubical volume 1 × 1× 1 filled with 64 thousand spheres of relative diameter 0.05, the coordination number N comes to 6.11–6.14 and the voidage ε, to about 0.40.

3. For the analysis of the properties of a packing, the use of a unit square section and cubical volume is substantiated, which makes it possible to narrow the region of investigation of the skeleton structure in mathematical simulation of the problems of bed conductivity. It has been established on their basis that the elementary volume that reflects the integral characteristics of the bed (voidage and coordination number) is of the order of about $200d^3$. The size of the elemental area is (12 × 12)d. The depth of the wall region within which the properties of the packing differ from the properties of the bed core is equal to about 1.5d.

NOTATION

d, diameter of a spherical particle, m; D, size of an elemental area, units of d; $\mathbf{F}_g$, vector of gravity force, H; $\Sigma\mathbf{F}$, resulting vector of forces acting on a sphere, N; $f(N)$, probability distribution function of the coordination number; $g(R)$, radial function of random filling; G, specific electrical conductivity of material, S/m; G_0, specific electrical conductivity of the bed, S/m; h_r, roughness of the material surface, mm; K, proportionality factor taking into account the elastic properties of granular system; L, linear dimension of the elementary volume, units of d; N, coordination number (the number of contacts of a particle with neighboring particles); N^*, number of neighboring spheres; Δn, relative displacement of a sphere in packing; P, load of a bed, Pa; r, relative radius of a sphere; S, displacement of the area, units of d; x, y, z, relative coordinates of a sphere; y_1, relative radius of the actual spot of a contact with account for the surface roughness; y_4, relative radius of the averaged element of the bed; Δ, distance between the centers of spherical particles in relative units; δ, error of calculations, %; ε_f, transparency (the ratio of the area of a gap to the total area of the bed section); ε, voidage (ratio of the total volume free of particles to the bed volume); Λ, relative electrical conductivity of a bubbling bed; φ, density of the packing of particles (ratio of the total volume of particles to the volume of the bed); Ω, specific electrical resistance, Ω·cm. Indices: r, roughness; f, free; g, gravitation; i, j, numbers of a current sphere and of a set of packed spheres.

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