SIMULATION OF THE STRUCTURE AND CALCULATION OF THE THERMAL CONDUCTIVITY OF POLYDISPERSED GRANULAR SYSTEMS

D. P. Volkov and Yu. P. Zarichnyak

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We propose a model and an approximate method for the calculation of the thermal conductivity of a free packing of polydispersed granular systems.

The complexity of the geometric simulation of a disordered structure of granular systems and the purely mathematical difficulties of the subsequent description of the effective transfer coefficients in such systems are probably the reason that the model studies we know of in this field are devoted to the investigation [1-4] of "monodispersed" structures with dimensions of unelongated particles which differ little from one another. The structure of the system is usually simulated by ordered or disordered agglomerations of spheres of equal dimensions. The minimum attainable porosity P_{min} of known monodispersed models of spherical particles lies in the range $0.26 \leqslant P_{min} \leqslant 0.47$, depending on the type of agglomeration of the grains. At the same time, the porosity of real polydispersed packings of grains used for reactor fuel elements [5] and structural materials used in the latest technology [6] lies in the range $0.05 \leqslant P_{min} \leqslant 0.3$. Such granular materials constitute a natural "polydispersed" structure (or an artificially produced one for special purposes) with differences of an order of magnitude or more between the dimensions of the component grains.

Our sample estimates of the possibility of calculating the effective thermal conductivity of a "polydispersed" packing of grains on the basis of relations obtained for monodispersed structures (e.g., by the method of successive reduction of a polydispersed structure to a monodispersed one) indicate that the calculated values are systematically higher than the experimental ones by ~60-100%, which is much higher than the measurement error.

Formulation of the Problem. We propose a model of the structure of polydispersed grains and an approximate method for calculating the effective thermal conductivity. We describe the methodology by using the example of the study of the thermal conductivity of a disordered polydispersed structure formed by a mixture of three collections of grains which differ markedly in dimension, $d_I \gg d_{II} \gg d_{III}$ (adjacent diameter values differ by a factor of 6-10). A schematic depiction of the structure of the polydispersed grains is shown in Fig. 1. Using the experience of earlier investigations [2], we introduce a geometric hierarchy in the system under study. The portions of the volume which are filled with particles having the smallest average dimension d_{III} will be called the "third-rank" structure. Together with the larger particles of dimension d_{II}, they form the "second-rank" structure, which fills the entire volume of the system not occupied by the particles with the largest dimension d_I. The second-rank structure and the large particles together form the "first-rank" structure.

Earlier [2] it was shown that if the porosity P of a structure of any rank exceeds 0.4, then the structure itself is a combination of a skeleton made up of a relatively dense packing of particles (the "first-order" structure) and larger voids incorporated in it, the two making up the "second-order" structure.

The fine particles in the polydispersed material occupy those cavities whose dimension is greater than or equal to the dimension of the fine particles, i.e., $l \geqslant d_i$. Therefore, in the zone of contact of the larger particles there remain gaps — "cuffs" free of finer particles.

Initial Information. If grains with different average dimensions are formed from different materials, then we must know the thermal conductivities of these materials λ_1, λ_2, λ_3, the properties of the gas or liquid filling the pores λ_p (as a rule, $\lambda_p < \lambda_1, \lambda_2, \lambda_3$), and the average dimensions of the particles d_I, d_{II}, d_{III}.

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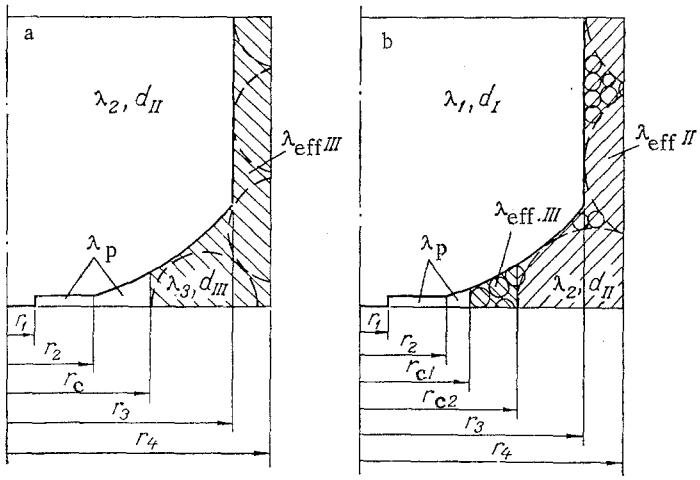

Fig. 1. Illustrating the determination of the thermal conductivity of polydispersed systems: a) element with averaged parameters of second-rank structure; b) element with averaged parameters of first-rank structure.

Scheme of Solution of the Problem. The calculation of the effective thermal conductivity of the polydispersed material is carried out by stages, beginning with the "lowest-rank" structure (in this case the third-rank structure). In the first stage, from the known values of the porosity of the third-rank structure (if the porosity is unknown, it can be estimated from the average particle dimension d_{III}) (Fig. 2) and the thermal conductivities of the particles and the material in the pores, λ_g and λ_p, we determine the effective thermal conductivity, λ_{eff}, of the monodispersed portion by any known method.

In the second stage the calculation is carried out on a modified model of a second-rank disordered structure. Figure 1b shows an element of a structure of this rank with averaged geometric parameters. The modification of the previously proposed model [2] consists in the fact that the space between the convex surfaces of the grains in the contact zone at a distance greater than the radius of the cuff is filled with a quasihomogeneous substance which has a thermal conductivity equal to the effective thermal conductivity of the third-rank structure, i.e., when $r < r_c$, we have $\lambda_{p.II} = \lambda_p$ and when $r \geqslant r_c$, we have $\lambda_{p.II} = \lambda_{eff.III}$. The boundaries of the region (the cuff) free of particles with dimension d_{III} are estimated from the geometric relations (Fig. 1):

$$r_c = \sqrt{2r_{II}r_{III} + r_{III}^2} - r_{III}. \tag{1}$$

Using methods for the approximate description of the heat-transfer process, we can obtain a formula for calculating the thermal conductivity of the skeleton of the second-rank structure:

$$\lambda_{skII} = f(\lambda_2,\ \lambda_{eff\,III},\ \lambda_p,\ P_{II},\ r_{II},\ r_{III}) = \tag{2}$$

$$= \frac{\lambda_2}{y_4^2}\left[\frac{y_1^2}{h + (1-h)\Phi} + \frac{y_2^2 - y_1^2}{h/\nu + 1 - h} + \frac{2\nu C}{1-\nu} + \frac{2\nu_1 D}{1-\nu_1} + \nu_1(y_4^2 - y_3^2)\right],$$

where

$$C = Q_1 - Q_2 + A\ln\frac{A - Q_1}{A - Q_2};\quad A = \frac{1}{1-\nu};\quad \nu = \frac{\lambda_p}{\lambda_2};$$

$$D = Q_3 - Q_1 + B\ln\frac{B - Q_3}{B - Q_1};\quad B = \frac{1}{1-\nu_1};\quad \nu_1 = \frac{\lambda_{eff\,III}}{\lambda_2};$$

$$Q_1 = \sqrt{1 - y_c^2};\quad Q_2 = \sqrt{1 - y_2^2};\quad Q_3 = \sqrt{1 - y_3^2}.$$

$$y_c = \frac{r_c}{r_{II}};\quad y_i = \frac{r_i}{r_{II}}\ (i = 1,\ 2,\ 3,\ 4)$$

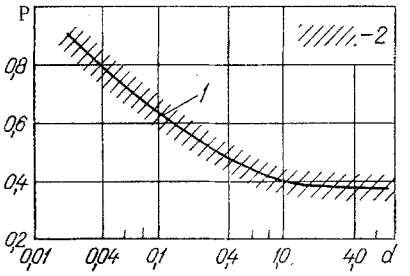

Fig. 2. Porosity of loose packing of granular systems as a function of the average particle dimension: 1) averaged curve; 2) zone of dispersion of the experimental data. d, mm.

(the relative radii of an element with averaged parameters) are found from the expression (1) and the formulas given in [2]. The effective thermal conductivity of the second-rank structure can be determined by the formula for structures with interpenetrating components, which in the case considered here takes the form

$$\lambda_{\text{eff II}} = \lambda_{\text{sk II}} [c_2^2 + \nu_{\text{sk}}(1-c_2)^2 + 2\nu_{\text{sk}} c_2 (1-c_2)(\nu_{\text{sk}} c_2 + 1 - c_2)^{-1}], \quad \nu_{\text{sk}} = \lambda_{\text{eff III}}/\lambda_{\text{sk II}}, \tag{3}$$

where c_2 is a geometric parameter of the skeleton which is related to the porosity of the second-rank structure by an equation of the type

$$P_{\text{II}} = 2c_2^3 - 3c_2^2 + 1. \tag{4}$$

In the last stage we find the effective thermal conductivity of the entire system $\lambda_{\text{eff.I}} = \lambda$. Figure 1b shows an element of a first-rank structure with averaged geometric parameters. The zone of contact between the particles in the structure of this rank is filled with quasihomogeneous substances having different thermal conductivities, i.e., when $r < r_{c1}$, we have $\lambda_{p.I} = \lambda_p$, when $r_{c1} \leqslant r \leqslant r_{c2}$, we have $\lambda_{p.I} = \lambda_{\text{eff.III}}$, and when $r > r_{c2}$, we have $\lambda_{p.I} = \lambda_{\text{eff.II}}$. The dimensions of the cuffs free of particles, r_{c1}, and those filled with a substance having thermal conductivity $\lambda_{\text{eff.III}}$, r_{c2}, are determined from formulas analogous to (1):

$$r_{c1} = \sqrt{2r_I r_{\text{III}} + r_{\text{III}}^2} - r_{\text{III}}, \tag{5}$$

$$r_{c2} = \sqrt{2r_I r_{\text{II}} + r_{\text{II}}^2} - r_{\text{II}}. \tag{6}$$

The expression for the calculation of the effective thermal conductivity of the entire system will have the form

$$\lambda_{\text{eff I}} = f(\lambda_1, \lambda_{\text{eff II}}, \lambda_{\text{eff III}}, \lambda_p, P_I, r_I, r_{\text{II}}, r_{\text{III}}) =$$

$$= \frac{\lambda_1}{y_4^2}\left[\frac{y_1^2}{h + (1-h)\Phi} + \frac{y_2^2 - y_1^2}{h/\nu + 1 - h} + \frac{2\nu C}{1-\nu} + \frac{2\nu_1 D}{1-\nu_1} + \frac{2\nu_2 E}{1-\nu_2} + \nu_2(y_4^2 - y_3^2)\right], \tag{7}$$

where

$$C = Q_1 - Q_2 + A \ln \frac{A - Q_1}{A - Q_2}; \quad A = \frac{1}{1-\nu}; \quad \nu = \frac{\lambda_p}{\lambda_1};$$

$$D = Q_3 - Q_1 + B \ln \frac{A - Q_3}{A - Q_1}; \quad B = \frac{1}{1-\nu_1}; \quad \nu_1 = \frac{\lambda_{\text{eff III}}}{\lambda_1};$$

$$E = Q_4 - Q_3 + F \ln \frac{F - Q_4}{F - Q_3}; \quad F = \frac{1}{1-\nu_2}; \quad \nu_2 = \frac{\lambda_{\text{eff II}}}{\lambda_1};$$

$$Q_1 = \sqrt{1 - y_{c1}^2}; \quad Q_2 = \sqrt{1 - y_2^2}; \quad Q_3 = \sqrt{1 - y_{c2}^2}; \quad Q_4 = \sqrt{1 - y_3^2};$$

$$y_{c1} = \frac{r_{c1}}{r_I}; \quad y_{c2} = \frac{r_{c2}}{r_I}, \quad y_i = \frac{r_i}{r_I} \quad (i = 1, 2, 3, 4).$$

TABLE 1. Thermal Conductivity of Polydispersed Granular Systems

Packing components and particle diam. d, in m	Concn. of components by volume	Thermal conductivity, W/m·deg K			$\frac{\lambda_{exp}-\lambda_{calc}}{\lambda_{exp}} \times 100\%$
		components	expt.	calc.	
Steel ($2.5 \cdot 10^{-3}$) + air	0,592 0,408	48 0,0264	0,5	0,44	+12
Steel ($2.5 \cdot 10^{-3}$) + bronze ($0.35 \cdot 10^{-3}$) + air	0,592 0,202 0,206	48 29 0,0264	0,9	1,1	—22
Steel ($2.5 \cdot 10^{-3}$) + bronze ($0.35 \cdot 10^{-3}$) + iron ($0.05 \cdot 10^{-3}$) + air	0,592 0,202 0,045 0,161	48 29 77 0,0264	1,2	1,48	—23
Steel ($3.2 \cdot 10^{-3}$) + air	0,557 0,443	48 0,0264	0,45	0,42	+6,7
Steel ($3.2 \cdot 10^{-3}$) + bronze ($0.35 \cdot 10^{-3}$) + air	0,557 0,171 0,272	48 29 0,0264	0,8	0,87	—8,8
Steel ($3.2 \cdot 10^{-3}$) + bronze ($0.35 \cdot 10^{-3}$) + copper ($0.005 \cdot 10^{-3}$) + air	0,557 0,171 0,038 0,234	48 29 395 0,0264	1,2	1,01	+15,8
Bronze ($0.35 \cdot 10^{-3}$) + air	0,608 0,392	29 0,0264	0,4	0,38	+2,5
Bronze ($0.35 \cdot 10^{-3}$) + copper ($0.005 \cdot 10^{-3}$) + air	0,608 0,117 0,274	29 395 0,0264	0,7	0,68	+2,9

Let us estimate the expected error in the calculation by the proposed method. As was shown in [2], on large bodies of experimental data (200-300 points) the discrepancy between the theoretical and measured values of the effective thermal conductivity of monodispersed granular systems was between 5% and 20% (the mean-square deviation was about 10%). Taking account of the fact that the calculation of the effective thermal conductivity of polydispersed systems is carried out stage by stage, the error in the calculation of the thermal conductivity of lower-rank structures in the first stage will make a certain contribution to the error in the calculation of the properties of the higher-rank structure in the next stage.

However, experience with the stage-by-stage calculation of the effective properties of multicomponent systems (up to eight components) [2] shows that the random errors in the calculation at different stages will partly compensate each other, so that the error will increase only slightly. Therefore, we may assume that the expected discrepancy between calculation and experiment for polydispersed structures made up of a mixture of grains of two or three average dimensions will lie in the 5-25% range, with a mean-square deviation of about 15%.

Results of the Calculation and Comparison with the Experimental Data. To verify the domain of applicability of the model developed here and the approximate method of calculation and error estimation, we measured the effective thermal conductivities of polydispersed structures of different ranks. The experimental investigations were carried out on an apparatus designed at the Thermophysics Department of the Leningrad Institute of Precision Mechanics and Optics. The measurement error was about 10%, and the measurement results were compared with the calculated values (see Table 1).

As was to be expected, the measurement results differ from the calculations by 15% on the average and exhibit qualitative and quantitative agreement between theory and experiment within the limitations of the approximation considered.

It should be emphasized that the proposed model and calculation method are designed for granular packings in which the volume of the grains V_g in the lower-rank structure (i + 1) is less than or equal to the volume of the pores V_p in the higher-rank structure (i), that is to say, $V_{g.i+1} \leqslant V_{p.i}$. Polydispersed granular systems in which $V_{g.i+1} > V_{p.i}$ constitute a separate class of structures. The methods of calculating the effective properties of such systems and combined structures form the subject of an independent investigation.

The results obtained can be used for predicting the effective thermal conductivity of polydispersed (two-component and multicomponent) granular systems and for developing programs for the experimental investigation, monitoring, analysis, and generalization of the measurement results.

NOTATION

P, porosity of the packing; d_I, d_{II}, d_{III}, average particle diameters; r_I, r_{II}, r_{III}, average particle radii; λ_1, λ_2, λ_3, λ_p, thermal conductivities of the grains and the component in the pores; r_c, r_{c_1}, r_{c_2}, radii of "cuffs"; $\lambda_{eff.III}$, $\lambda_{eff.II}$, $\lambda_{eff.I}$, effective thermal conductivities of intermediate fractions and of the entire system; $\lambda_{sk.II}$, thermal conductivity of the skeleton; y_c, y_{c_1}, y_{c_2}, y_1, y_2, y_3, y_4, relative radii of element with averaged parameters; V_g, V_p, volumes of the grains and the pores; h, Φ, height of the microroughness of the grains and heat flux spreading function (determined by formulas from [2]).

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CALCULATION OF THE THERMAL CONDUCTIVITY OF HETEROGENEOUS MATERIALS WITH DISORDERED STRUCTURE

V. A. Osipova and Kh. A. Kyaar

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Structural models for determining the effective transport coefficients for two-component heterogeneous materials are analyzed and the results are compared with experimental data.

The problem of calculating the thermal conductivity of heterogeneous materials with the help of the theory of generalized conductivity is still an important problem, in spite of the progress made [1, 2]. The development of new technologies for obtaining heterogeneous materials greatly increases the range of possible structures, whose neglect can lead to large errors in determining conductivity.

It should be noted that sometimes this structural dependence of the conductivity is not used correctly: secondary properties are chosen as a foundation for the new model and for the computed characteristics [3]. The classical starting information for calculating the characteristics determining the conductivity includes the volume fractions (m_1, m_2) and coefficients of thermal conductivity of the components (λ_1, λ_2). We will examine heterogeneous materials consisting of two solid components and we will estimate the accuracy that we can expect for the computational results. If it is assumed that the coefficients of thermal conductivity of the components are known to within ~10% and the volume fractions to within 5%, then a calculation using the equation for a structure with cubic isolated inclusions [2]

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