EFFECTIVE THERMAL CONDUCTIVITY OF DISPERSE MEDIA AT SMALL PECLET NUMBER

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The steady heat conduction of disperse media consisting of identical spherical particles is calculated for small Peclet numbers characterizing the heat transfer at the level of the individual particles; heat transfer by contact conduction over the disperse phase is neglected.

The theoretical investigation of the thermophysical, electrodynamic, and other properties of heterogeneous materials containing discrete particles of a disperse phase began with Maxwell [1] and Rayleigh [2], and the number of papers in this field is very large (see the reviews [3-6]). The most popular lines of research are represented by the theories of [7-10]; more recent data are described in [3-6] and also in [11-14]. Essentially, however, accurate results have only been obtained for the effective characteristics of dilute systems, in which the volume content of particles is low. Generalizations to concentrated systems are based on more or less plausible hypotheses as to the influence of individual particles or groups of particles on the mean field of thermodynamic forces and currents in the disperse medium and on attempts to find an approximate statistical description of the perturbations introduced by the particles. More rigorous problems involving such perturbations may be formulated within the framework of the general theory of [15]. We emphasize that the problem of determining the macroscopic coefficients of thermal conductivity or diffusion characteristic of the disperse medium as a whole from the known properties of the phases that it contains, and its microstructure, is a particular case of the more general problem of describing transfer processes in heterogeneous materials, discussed in [16].

We consider a disperse medium containing spherical particles of identical size and properties. The Peclet number, characterizing the convective heat transfer inside and outside the individual particles, is assumed to be small in comparison with unity, so that it is possible to neglect the effect of random phase pulsations and also of regular motion associated with the mean flow of continuous phase past the particles. In addition, we neglect the conductive heat transfer over the disperse phase caused by direct contact between particles. (These contacts occur, generally speaking, not only in densely packed systems with motionless particles of granular-bed type, or in concentrated composite materials, but also in systems with pulsating particles of fluidized-bed type). Then, under steady conditions, when there is no heat transfer between the phases and their mean temperatures τ_0 and τ_1 are equal to the mean temperature τ of the medium as a whole, we write the equation [15]

$$\nabla \mathbf{q} = 0, \quad \mathbf{q} = -\lambda_0 \nabla \tau - (\lambda_1 - \lambda_0) \langle (1-\theta) \nabla T \rangle \tag{1}$$

in a coordinate system fixed in the medium; in this equation

$$\langle (1-\theta) \nabla T \rangle = n(\mathbf{r}) \int\limits_{x=a} \tau^* (\mathbf{r} + \mathbf{x} \mid \mathbf{r}) \mathbf{n} d\mathbf{x}, \tag{2}$$

the integration being taken over the surface of a specimen particle of the medium with center at the point $\mathbf{r}$, at which the mean temperature is τ^* (the notation of [15] is employed). The vector defined in Eq. (2) should be a linear function of the vector $\nabla\tau$ characterizing the anisotropy of the heat-conduction process, i.e., we may write

$$\langle (1-\theta) \nabla T \rangle = \rho \nu \nabla \tau, \quad \mathbf{q} = -\lambda \nabla \tau, \quad \lambda = \lambda_0 + (\lambda_1 - \lambda_0) \rho \nu, \tag{3}$$

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where ν is an unknown coefficient depending on ρ and the thermal conductivity of the phases, while λ acts as the effective thermal conductivity of the disperse medium; both these parameters may be calculated from Eq. (2) if the temperature τ^* is known. Note that in the above discussion it was assumed implicitly that the linear scale of the mean characteristics of the medium (for example, its concentration) is significantly larger than the scale of the temperature field, so that the vector $\nabla\rho$ determining the anisotropy of the medium itself may, in general, be excluded from consideration.

To determine the temperature inside the specimen particle we consider the perturbations that it produces in the mean temperature field of the medium, which we write in the form $\tau = \mathbf{Er}$. An approximate formulation of this problem follows, for example, from the method proposed in [15] of closing an infinite chain of equations describing a temperature field perturbed by many particles. Taking the origin of the coordinates at the center of the specimen particle, for the mean temperature τ_0^* of the continuous phase close to the particle we have the problem

$$\nabla[B(r)\nabla\tau_0^*] = 0,\ r > a;\ \Delta\tau^* = 0,\ a > r \geqslant 0,$$
$$\nabla\tau_0^* \to \mathbf{E},\ r \to \infty;\ \tau^* < \infty,\ r = 0, \tag{4}$$
$$\tau_0^* = \tau^*,\ B(a)\,\mathbf{n}\nabla\tau_0^* = \lambda_1 \mathbf{n}\nabla\tau^*,\ r = a,$$

where

$$B(r) = \lambda_0\beta(\xi),\ \beta(\xi) = 1 + (\varkappa - 1)\rho\nu\sigma(\xi),\ \xi = \frac{r}{a},\quad \varkappa = \frac{\lambda_1}{\lambda_0}, \tag{5}$$

while, on the basis of [15], the function $\sigma(\xi)$ may be represented in the following form:

$$\sigma(\xi) = \frac{27 - 56\xi + 30\xi^2 - \xi^4}{16\xi},\ 1 < \xi < 3,$$
$$\sigma(\xi) = 1,\ \xi > \zeta. \tag{6}$$

It is evident that $\sigma(1) = 0$, so that $B(a) = \lambda_0$; for $\xi > 3$, $B(r) = \lambda$.

Formally, Eq. (4) corresponds to the idea that the specimen particle is immersed in some hypothetical homogeneous medium, the effective thermal conductivity of which is $B(r)$, i.e., depends on the distance to the surface of the particle. For a medium of low concentration, it is permissible, in general, to ignore the dependence in Eq. (6), i.e., to take $\sigma(\xi) = 1$. This amounts to not taking into account that the particles cannot interpenetrate, i.e., that the centers of adjacent particles cannot be less than $2a$ apart. For a concentrated medium, $\sigma(\xi)$ may be approximated by a step function which is zero for $\xi < 2$ and unity for $\xi > 2$. This corresponds to a specimen particle immersed in a hypothetical homogeneous medium which is separated from the surface of the particle by a spherical layer filled with a pure continuous phase. The idea of such a layer was first introduced in [17], on the basis of phenomenological considerations. However, the thickness of this layer is a and is independent of the concentration; this is contrary to the usual assumption, characteristic for cell models, which was used, for example, in [5, 13], in calculating the effective thermal conductivity. The solution of Eq. (4), under the given simplifying assumptions, was obtained in [14].

The formulation in Eq. (4) of the specimen-particle problem has a fundamental deficiency in that the mean temperature and the heat flow, which, in general, should not depend on fixing the center of the particle at a given point, are found to be formally related by the expression $\mathbf{q} = -B(r)\nabla\tau$, which disagrees with the analogous relation in Eq. (3). It is clear from elementary considerations that this relation, which refers to the disperse medium as a whole, should not be sensitive to the position and choice of the specimen particle, which can only affect the character of the perturbation $\tau' = \tau_0^* - \tau_0$ of the mean temperature field and not the field itself. Therefore, the specimen-particle problem should only be formulated for this perturbation, with respect to which the particle surface acts as an external boundary. The statement of the problem is easily obtained by the general method of [15]. Omitting the details of the derivation, we write the final result:

$$\nabla[B(r)\nabla\tau'] = 0,\ r > a,\ \Delta\tau^* = 0,\ a > r \geqslant 0,$$
$$\tau' \to 0,\ r \to \infty,\ \tau^* < \infty,\ r = 0, \tag{7}$$
$$\tau' + \mathbf{Er} = \tau^*,\ \lambda_0 \mathbf{n}\nabla\tau' + \lambda\mathbf{nE} = \lambda_1 \mathbf{n}\nabla\tau^*,\ r = a,$$

the function $B(r)$ being determined as before from Eq. (5).

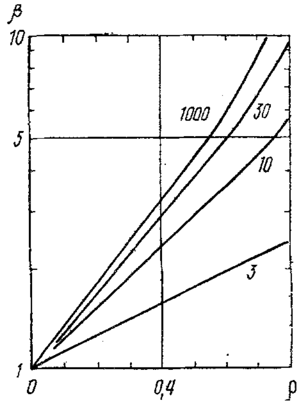

Fig. 1

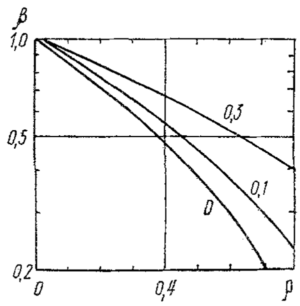

Fig. 2

Fig. 1. Concentration dependence of dimensionless thermal conductivity β of medium for various $\varkappa$ (numbers on the curves).

Fig. 2. Value of β as a function of ρ for small $\varkappa$ (numbers on the curves).

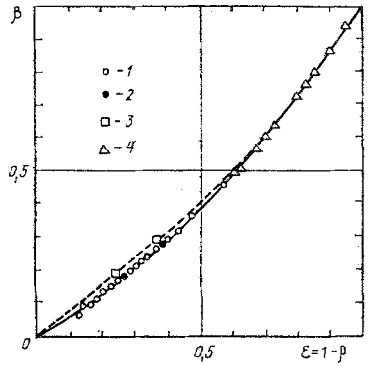

Fig. 3. Comparison of results obtained from Eq. (12) for $\varkappa$ = 0 (continuous curve) with experimental data of [13, 18-20]: 1) [18]; 2) [13]; 3) [19]; 4) [20]; the dashed line corresponds to the formula in [5, 13].

The boundary-value problem in Eq. (7) may be considerably simplified if it is taken into account that the angular dependences of τ' and τ^* are contained in the factor $\mathbf{Er}$. Then Eq. (7) reduces to a two-point problem for ordinary differential equations with the independent variable r; the parameter ν acts as an eigenvalue of the problem, for the determination of which there is a "superfluous" boundary condition. A special numerical method will be developed for the solution of this eigenvalue problem.

To obtain the result in analytical form, the following approximation is used:

$$\sigma(\xi) = \begin{cases} 0, & \xi < 2, \\ 1, & \xi > 2, \end{cases} \quad B(r) = \begin{cases} \lambda_0, & r < 2a, \\ \lambda, & r > 2a. \end{cases} \tag{8}$$

Then the expression for $r > a$ in Eq. (7) leads to the Laplace equation for the temperature in the regions $a < r < 2a$ and $r > 2a$; the thermal conductivities in these regions are λ_0 and λ, respectively, and at their boundaries the usual continuity conditions apply for the temperature and the normal component of the heat flow. The solution of this problem is obtained by standard means and takes the form

$$\tau' = \begin{cases} A\left(\frac{a}{r}\right)^3 \mathbf{Er}, & r > 2a, \\ \left[A'\left(\frac{a}{r}\right)^3 + C'\right]\mathbf{Er}, & a < r < 2a, \end{cases} \qquad \tau^* = C\mathbf{Er}, \tag{9}$$

where

$$A = -\frac{12}{D}(\varkappa - \beta), \quad C = \frac{1}{D}(7\beta^2 + 22\beta + 7),$$

$$A' = -\frac{4}{D}(\varkappa - \beta)(2\beta + 1), \quad C' = \frac{1}{D}(\varkappa - \beta)(\beta - 1), \tag{10}$$

$$D = \beta(7\varkappa + 17) + 5\varkappa + 7, \quad \beta = \beta(\infty) = 1 + (\varkappa - 1)\rho\nu, \quad \varkappa = \frac{\lambda_1}{\lambda_0}.$$

Here the dimensionless parameters $\varkappa$ and β are used for the thermal conductivity, and the parameter ν introduced in Eq. (3) coincides with C. The formal representation of λ can be obtained from Eqs. (3) and (10):

$$\lambda = \lambda_0 + (\lambda_1 - \lambda_0)(7\beta^2 + 22\beta + 7)[\beta(7\varkappa + 17) + 5\varkappa + 7]^{-1}\rho. \tag{11}$$

Dividing Eq. (11) by λ_0, we obtain an equation for β; its solution

$$\beta = [7\varkappa(1-\rho) + 17 + 7\rho]^{-1}\{\varkappa(1 + 11\rho) + 5 - 11\rho + ([\varkappa(1 + 11\rho) + 5 - 11\rho]^2 + [7\varkappa(1-\rho) + 17 + 7\rho][\varkappa(5 + 7\rho) + 7(1-\rho)])^{1/2}\} \tag{12}$$

finally determines the effective thermal conductivity of the disperse medium.

The dependence of β on ρ is shown in Fig. 1 for $\varkappa > 1$ (i.e., for media containing particles of higher thermal conductivity) and in Fig. 2 for $\varkappa < 1$ (i.e., for media with poorly conducting inclusions). In order to improve the accuracy of Eq. (12), which is based on the model approximation in Eq. (8), we performed a direct numerical solution of Eq. (7) for individual values of $\varkappa$ and ρ, using a BÉSM-4 computer. In all cases, the discrepancy in the results for β did not exceed 4-5%.

Since many other empirical and model relations have been proposed for the effective thermal conductivity of disperse media, it is particularly important to make a thorough comparison of Eq. (12) with experimental data. In concentrated media with heat-conducting inclusions, contact heat transfer directly between the particles may play a significant role, and therefore the theory was compared mainly with data referring to situations where $\varkappa < 1$, i.e., with experimental data on the diffusion of impurities in a granular bed with practically impermeable particles, on heat conduction in porous materials, and on the electrical conduction of mixtures with nonconducting inclusions, also lacking surface conduction by solvated shells, etc. The results of the comparison provide persuasive support for Eq. (12), although in a number of cases the difference from other formulas is very slight. An example of the comparison of theoretical curves corresponding to Eq. (12) for $\varkappa = 0$ with experimental data from [13, 18-20] is shown in Fig. 3, where the dashed line shows a curve derived from one of the best-known formulas, obtained in [5, 13].

For $\varkappa \gg 1$ and large ρ, the results given by Eq. (12) are too low. This is a result of neglecting contact heat conduction. In principle, contact heat conduction may be taken into account by considering simultaneously the heat transfer of a specimen particle with two coexisting hypothetical media that model phases of the medium and have, in general, different mean temperatures. Using the superposition principle, the theory can easily be extended to cover polydisperse media and media containing particles of different thermal conductivities. The analysis of these factors involves simple but rather cumbersome additional calculations and falls outside the scope of the present work.

NOTATION

A, A'	are the coefficients in Eqs. (9) and (10);
a	is the particle radius;
B(r)	is the function defined in Eq. (5);
C, C', D	are the coefficients in Eqs. (9) and (10);
E	is the mean temperature gradient of medium;
n	is the countable particle concentration;
n	is the unit vector along external normal;
r	is the radius-vector;

$\beta = \lambda/\lambda_0$; $\beta(\xi)$	is the function in Eq. (5);
$\varkappa = \lambda_1/\lambda_0$; λ	is the thermal conductivity;
ν	is the parameter introduced in Eq. (3);
ξ	is the dimensionless variable from Eqs. (5) and (6);
ρ	is the volume concentration of particles;
$\sigma(\xi)$	is the function defined in Eq. (6);
τ	is the mean temperature.

Indices

0 is the continuous phase;
1 is the disperse phase;
* is the temperature inside and outside specimen particle.

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