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A rigorous derivation of the equations of heat transport is carried out by averaging over an ensemble for a system consisting of a continuous medium with particles imbedded in it, and the closure problem for these equations is discussed.

A usual situation in engineering practice is one where the linear scale L of the measurements of the significant quantities characterizing the mean "macroscopic" properties of a dispersed medium and of the transport processes in it is considerably larger than the scale l of the internal structure of the medium. In this case, it is natural to consider the transport of heat or mass as occurring in some homogeneous continuum (or in several homogeneous continua coexisting simultaneously at each point of space occupied by the medium) which is an abstraction of the "microscopic" features of transport in the neighborhood of individual particles. Two interrelated problems arise as a result: the derivation of effective transport equations in such continua and their closure, i.e., the representation of all terms appearing in them in the form of functions of the unknown variables in these equations and of quantities describing the structure of the medium and the physical properties of its phases. Similar problems also arise in the formulation of rheological models for dispersed media, in studies of stress and strain fields in composite materials, and in the analysis of electromagnetic fields in dispersed conductors and dielectrics.

The first problem is gotten around most often by a priori postulation of equations for one-dimensional transport in dispersed and other heterogeneous media [1-4] or for their three-dimensional analogs [5]. Such an approach leaves open questions about the adequacy of the equations or the conditions for their applicability and questions about the method for calculating the coefficients appearing in them, which can only be obtained experimentally in this situation (for example, see the review in [6]). Sometimes such equations are formulated by averaging the local equations of thermal conductivity or diffusion valid in the separate phases over representative volumes of the medium [7-10]. In this case also, however, the derivation of the equations contains only the most general indications of the method for determination of the unknown terms in them; besides, it is necessary to assume additional ergodic hypotheses about the equivalence of averaging over volume and averaging over a surface, etc., the validity of which is not obvious beforehand. Therefore, the rigorous derivation, justification, and analysis of macroscopic transport equations, including those widely used in practice, remain an unsolved problem thus far. The powerful apparatus of ensemble averaging is drawn on for a study of this problem in the following.

We consider a dispersed medium consisting of a continuous phase and a dispersed phase of particles distributed in it. In the general case, both phases of the medium are mobile and its concentration is not necessarily small. For simplicity, the particles are assumed to be identical spheres; generalization to a system of varying particles presents no fundamental difficulties but leads to more cumbersome computations. Examples of such media are suspensions and emulsions, fluidized and fixed beds of spherical particles, granular composite materials, etc.

Within the continuous and dispersed phases, the usual equations of convective thermal conductivity are valid and can be written in the form

$$C \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \right) T = -\nabla \mathbf{Q} \cdot \mathbf{H}, \quad \mathbf{Q} = -\Delta \nabla T, \quad (1)$$

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where the "detailed" thermal conductivity and heat capacity per unit volume are determined through phase parameters by means of the expressions

$$\Lambda = \theta\lambda_0 + (1 - \theta)\lambda_1, \quad C = \theta c_0 + (1 - \theta)c_1, \quad (2)$$

where θ is a structure function which is equal to one in the spaces between particles and to zero inside them. The problem involves averaging of (1) in order to obtain equations for the mean temperatures of the phases considered as homogeneous continuous media.

According to the general Gibbs method, the most proper averaging is over an ensemble of possible states of the dispersed medium where in the most general case the states are distinguished both by the positions of the centers of the particles and by their translational and rotational velocities. Correspondingly, the detailed fields T , V , and other detailed functions depend not only on coordinates and time, but also on the state realized. In first approximation, the dependence on velocities can be neglected by considering states corresponding to an identical set of vectors $\mathbf{r}^{(i)}$, but with different $d\mathbf{r}^{(i)}/dt$, for example, as indistinguishable.† We then arrive at the concept of an ensemble of configurations, the phase space of which is formed by components of the vectors $\mathbf{r}^{(i)}$ and has the dimensionality $3N$. In accordance with the usual ergodic conditions, we assume that ensemble means coincide with the quantities which are obtained by averaging over volumes containing a sufficiently large number of particles.

We introduce the distribution function $\varphi(t, A_N)$ for the configuration A_N , which is a probability density in phase space, and also the conditional distribution functions $\varphi(t, A_{N-1}|\mathbf{r}')$ and $\varphi(t, A_{N-2}|\mathbf{r}', \mathbf{r}'')$ for configurations in which the positions \mathbf{r}' and \mathbf{r}'' for one or two particles are fixed. The corresponding unconditional and conditional means for any detailed function $G(t, \mathbf{r}|A_N)$ are then written in the form

$$\begin{aligned} g(t, \mathbf{r}) &= \langle G \rangle = \int G(t, \mathbf{r}|A_N) \varphi(t, A_N) dA_N, \\ g^*(t, \mathbf{r}|\mathbf{r}') &= \langle G \rangle^* = \int G(t, \mathbf{r}|A_N) \varphi(t, A_{N-1}|\mathbf{r}') dA_{N-1}, \\ g^{**}(t, \mathbf{r}|\mathbf{r}', \mathbf{r}'') &= \langle G \rangle^{**} = \int G(t, \mathbf{r}|A_N) \varphi(t, A_{N-2}|\mathbf{r}', \mathbf{r}'') dA_{N-2}, \end{aligned} \quad (3)$$

where the integrations are performed over phase spaces corresponding to ensembles of N , $N-1$, and $N-2$ particles. In view of the obvious equalities

$$\begin{aligned} \varphi(t, A_N) &= \varphi(t, \mathbf{r}') \varphi(t, A_{N-1}|\mathbf{r}'), \\ \varphi(t, A_{N-1}|\mathbf{r}') &= \varphi(t, \mathbf{r}''|\mathbf{r}') \varphi(t, A_{N-2}|\mathbf{r}', \mathbf{r}''), \end{aligned}$$

where $\varphi(t, \mathbf{r}')$ and $\varphi(t, \mathbf{r}'|\mathbf{r}'')$ are the unconditional (unary) and conditional (binary) distribution functions for a single particle, we have from Eqs. (3)

$$\begin{aligned} g(t, \mathbf{r}) &= \int g^*(t, \mathbf{r}|\mathbf{r}') \varphi(t, \mathbf{r}') d\mathbf{r}', \\ g^*(t, \mathbf{r}|\mathbf{r}') &= \int g^{**}(t, \mathbf{r}|\mathbf{r}', \mathbf{r}'') \varphi(t, \mathbf{r}''|\mathbf{r}') d\mathbf{r}''. \end{aligned} \quad (4)$$

Equations like (3) and (4) can also be written for configurations in which the locations of more than two particles are fixed. We emphasize that all distribution functions introduced are normalized to unity in their region of definition.

The means in Eqs. (3) refer to the dispersed medium as a whole. We introduce other means related to the continuous and dispersed phases:

$$\begin{aligned} \varepsilon g_0 &= \langle \theta G \rangle, \quad \rho g_1 = \langle (1 - \theta) G \rangle, \quad \varepsilon g_0 + \rho g_1 \equiv g, \\ \varepsilon^* g_0^* &= \langle \theta G \rangle^*, \quad \rho^* g_1^* = \langle (1 - \theta) G \rangle^*, \quad \varepsilon^* g_0^* + \rho^* g_1^* \equiv g^*, \\ \rho &= 1 - \varepsilon, \quad \varepsilon = \langle \theta \rangle, \quad \rho^* = 1 - \varepsilon^*, \quad \varepsilon^* = \langle \theta \rangle^*. \end{aligned} \quad (5)$$

We obtain a representation for the means over the dispersed phase needed in the following. For this purpose, we write

† This assumption is trivial for a system with fixed particles, but for the general case of a moving system it is a definite hypothesis deserving further investigation.

$$\theta(\mathbf{r}|A_N) = 1 - \sum_{i=1}^N \eta(a - |\mathbf{r} - \mathbf{r}^{(i)}|).$$

Here, η is a Heaviside function, and the summation is carried out over all particles. Using this expression and the concept of static indistinguishability of the particles, we have from Eqs. (3)-(5)

$$\langle (1 - \theta)G \rangle = N \langle \eta G \rangle = N \int \eta(a - |\mathbf{r} - \mathbf{r}'|) g^*(t, \mathbf{r}|\mathbf{r}') \varphi(t, \mathbf{r}') d\mathbf{r}' = N \int g^*(t, \mathbf{r}|\mathbf{r}') \varphi(t, \mathbf{r}') d\mathbf{r}', \quad |\mathbf{r} - \mathbf{r}'| \leq a.$$

The integration in the last integral is carried out over values of the radius vector \mathbf{r}' of the center of a particle such that the point \mathbf{r} is within that particle. Neglecting terms of the order of $a/L \ll l/L \ll 1$, one can replace $\varphi(t, \mathbf{r}')$ by the first term of its expansion in a Taylor series about the point \mathbf{r} and apply the parallel transport operator to the vector $\mathbf{x} = \mathbf{r} - \mathbf{r}'$ for the determination of g^* . We then obtain

$$\langle (1 - \theta)G \rangle = N \varphi(t, \mathbf{r}) \int_{x \leq a} g^*(t, \mathbf{r} + \mathbf{x}|\mathbf{r}) d\mathbf{x}. \quad (6)$$

In a similar fashion, an expression is obtained for the conditional means over the dispersed phase. We have

$$\langle (1 - \theta)G \rangle^* = N \int_{x \leq a} \varphi(t, \mathbf{r} + \mathbf{x}|\mathbf{r}') g^{**}(t, \mathbf{r}|\mathbf{r}', \mathbf{r} + \mathbf{x}) d\mathbf{x}. \quad (7)$$

The integration here is carried out over the volume of a particle with a center at the point \mathbf{r} (see Fig. 1).

Equations (6) and (7) make it possible to give a rigorous definition of the quantities ρ and ρ^* introduced in Eqs. (5), for which it is sufficient to set $G=1$. In the particular case of completely random arrangement of particles, the binary distribution function can be approximated by the relation

$$\varphi(t, \mathbf{r}|\mathbf{r}') = \varphi(t, \mathbf{r}) \eta(2a - |\mathbf{r} - \mathbf{r}'|). \quad (8)$$

In this case the integration in Eq. (7) is actually performed only over the portion of the volume of a particle with its center at \mathbf{r} which is shaded in Fig. 1. We then obtain for ρ and ρ^*

$$\rho(t, \mathbf{r}) = \frac{4}{3} \pi a^3 N \varphi(t, \mathbf{r}) = \frac{4}{3} \pi a^3 n(t, \mathbf{r}), \quad (9)$$

$$\rho^*(t, \mathbf{r}|\mathbf{r}') = \rho(t, \mathbf{r}) \sigma(\xi), \quad \xi = |\mathbf{r} - \mathbf{r}'|/a,$$

where σ is the ratio between the shaded volume in Fig. 1 and the volume of a sphere of radius a ; its dependence on ξ is shown in Fig. 2.

By definition, ensemble distribution functions are independent of \mathbf{r} and therefore the averaging operation and differentiation with respect to \mathbf{r} commute. Further, the time scale for detailed functions is determined by processes at the level of individual particles and is therefore much less than the time scale for the distribution functions, the variations of which are connected with regrouping of a large number of particles.† Therefore, to an accuracy of the order of quantities which are greater than the small ratio of the time scales specified, the averaging operation is also interchangeable with differentiation with respect to time, i.e.,

$$\left\langle \frac{\partial G}{\partial \mathbf{r}} \right\rangle = \frac{\partial}{\partial \mathbf{r}} \langle G \rangle, \quad \left\langle \frac{\partial G}{\partial t} \right\rangle = \frac{\partial}{\partial t} \langle G \rangle. \quad (10)$$

Similar commutation relations can also be written for the conditional means defined in Eqs. (3).

† This argument is invalid for systems with fixed particles and steady-state flow of the continuous phase where both scales tend toward infinity. In this case, however, $\varphi(t, \mathbf{r})$ is generally independent of t and the second equation in (10) is satisfied rigorously.

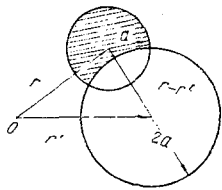


Fig. 1. Sketch illustrating integration in Eqs. (6) and (7) and the calculation of the function $\sigma(\xi)$ from Eq. (9).

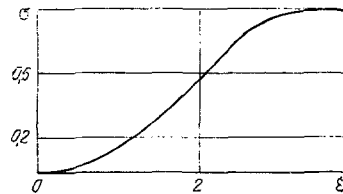


Fig. 2. Dependence of σ on ξ .

We now average Eq. (1) multiplied by θ and by $1-\theta$ with respect to the unconditional distribution function. Using Eqs. (2)–(5) and (10), and introducing the pulsations τ_0 , τ_1 , and \mathbf{v}_0 , \mathbf{v}_1 of the detailed fields T' and \mathbf{V}' with respect to their mean values in the respective phases, we obtain

$$\begin{aligned} \varepsilon c_0 \left(\frac{\partial}{\partial t} + \mathbf{v}_0 \frac{\partial}{\partial \mathbf{r}} \right) \tau_0 &= -c_0 \frac{\partial}{\partial \mathbf{r}} \langle \theta T' \mathbf{V}' \rangle - \nabla \mathbf{q} + \langle (1-\theta) \nabla \mathbf{Q} \rangle + \varepsilon h_0, \\ \rho c_1 \left(\frac{\partial}{\partial t} + \mathbf{v}_1 \frac{\partial}{\partial \mathbf{r}} \right) \tau_1 &= -c_1 \frac{\partial}{\partial \mathbf{r}} \langle (1-\theta) T' \mathbf{V}' \rangle - \langle (1-\theta) \nabla \mathbf{Q} \rangle + \rho h_1. \end{aligned} \quad (11)$$

Equations (11) describe heat transport in flows of the continuous and dispersed phases where the transport equation for the medium as a whole is the sum of Eqs. (11). On the left sides appear the rates of change of the heat content of the materials in the phases per unit volume of the medium, including convective heat transport by the mean flow. The first terms on the right sides are the divergences of the additional heat flows resulting from pulsational motion. In their significance, these "pulsational" flows are analogous, for example, to Reynolds stresses in the hydromechanics of turbulent flows, but their nature may be different depending upon the detailed structure of the medium and the pulsational mechanism. Thus, their occurrence may be associated with turbulence in the dispersed medium, with nonuniformity of local fluid velocity in the porous space of a granular bed, etc. The vector \mathbf{q} describes the "regular" mean heat flux in the medium resulting from molecular thermal conductivity including the perturbing effect of the dispersed particles on the temperature field in a continuous phase with a different thermal conductivity, and the quantity $\langle (1-\theta) \nabla \mathbf{Q} \rangle$ is the "regular" heat exchange between phases. Finally, the last terms on the right sides of Eqs. (11) describe the mean intensity of heat sources in the phase materials.†

For the determinacy of Eqs. (11), it is first of all necessary that the velocities \mathbf{v}_0 and \mathbf{v}_1 be known as well as ρ and other quantities characterizing the structure of the medium. In the general case, all these quantities are functions of t and \mathbf{r} which are determined from a solution of the independent problem of the motion of the dispersed medium or which are assigned a priori; they can be considered as known quantities in the following. All the remaining terms on the right sides of Eqs. (11) must be represented in the form of functions of the unknown variables τ_0 and τ_1 and also of the parameters characterizing the structure of the medium and the physical properties of the phases. It is apparent that the physical models required for such representation of the pulsational and regular terms are quite different in nature and must be considered separately. In the following, we limit ourselves to the analysis of the regular terms, neglecting heat sources for simplicity and assuming that pulsational thermal fluxes are small. The latter is completely valid in the very important case where the Péclet number, which is based on the characteristic particle size a and the mean velocity $|\mathbf{v}_0 - \mathbf{v}_1|$ of the flow around a particle, is small in comparison with one. In this case, we have in a coordinate system moving with a velocity \mathbf{v} instead of Eqs. (11)

$$\varepsilon c_0 \frac{\partial \tau_0}{\partial t} = -\nabla \mathbf{q} + \langle (1-\theta) \nabla \mathbf{Q} \rangle, \quad \rho c_1 \frac{\partial \tau_1}{\partial t} = -\langle (1-\theta) \nabla \mathbf{Q} \rangle. \quad (12)$$

Using Eq. (5) and the definition of \mathbf{Q} in Eq. (1), we have

$$\mathbf{q} = -\langle \Lambda \nabla T \rangle = -\lambda_0 \nabla T - (\lambda_1 - \lambda_0) \langle (1-\theta) \nabla T \rangle. \quad (13)$$

Thus, all the unknown terms in Eqs. (12) are means over the dispersed phase, which can be written in the form (6). In particular, using the Gaussian formula, we obtain from Eq. (6)

$$\begin{aligned} \langle (1-\theta) \nabla T \rangle &= n(t, \mathbf{r}) \oint_{x=a} \tau^*(t, \mathbf{r} + \mathbf{x}|\mathbf{r}) n d\mathbf{x}, \\ \langle (1-\theta) \nabla \mathbf{Q} \rangle &= n(t, \mathbf{r}) \oint_{x=a} \mathbf{q}^*(t, \mathbf{r} + \mathbf{x}|\mathbf{r}) n d\mathbf{x}, \end{aligned} \quad (14)$$

where the integration is performed over the surface of a particle with its center at \mathbf{r} . Consequently, Eqs. (12) will be closed if the mean temperature and the mean heat flux on the surface of an individual particle are known.

In order to determine the quantities mentioned, it is necessary to consider the problem of the mean perturbations introduced into the mean temperature fields of the phases by a test particle with a fixed location in the system. It is clear that the mean temperature within a particle satisfies the usual one-phase equation of

† Note that h_0 and h_1 also contain terms depending on T' in the case where H depends on temperature, and this dependence is nonlinear.

thermal conductivity. Equations for the fields τ_0^* and τ_1^* outside a particle are obtained after averaging Eq. (1) multiplied by θ or $1-\theta$; proceeding as in the derivation of Eqs. (11) and (12), for small Péclet numbers and $H=0$, we obtain in place of Eqs. (12) and (13)

$$\varepsilon^*c_0 \frac{\partial \tau_0^*}{\partial t} = -\nabla \mathbf{q}^* + \langle (1-\theta) \nabla \mathbf{Q} \rangle^*, \quad (15)$$

$$\rho^*c_1 \frac{\partial \tau_1^*}{\partial t} = -\langle (1-\theta) \nabla \mathbf{Q} \rangle^*, \quad \mathbf{q}^* = -\lambda_0 \nabla \tau^* - (\lambda_1 - \lambda_0) \langle (1-\theta) \nabla T \rangle^*.$$

The usual conditions for continuity of temperature and of the normal component of the heat flux must be satisfied at the surface of the test particle. The conditional means over the dispersed phase appearing in Eqs. (15) are expressed through conditional means of higher order in accordance with Eq. (7).

The determination of the latter means requires a solution of the problem of the mean perturbations introduced by two fixed particles, which can easily be formulated in analogy with the problem of a test particle. In this problem, terms appear which are expressed through the temperature fields averaged over configurations in which the positions of three particles are known beforehand. Continuing such a process, we obtain an infinite ($N \gg 1$) chain of interrelated problems for many particles. It does not seem possible to solve all these problems, and there then arises the problem of cutoff and closure of this chain, which is completely analogous to such problems in the statistical physics of fluids or in the statistical theory of turbulence.

The simplest version of closure, which was discussed in [10] in particular, was based on the following considerations. Because of the linearity of the equations of thermal conductivity, the quantities $\langle (1-\theta) \nabla T \rangle$ and $\langle (1-\theta) \nabla \mathbf{Q} \rangle$ must depend linearly on the temperatures τ_0 and τ_1 . The first of these quantities is a vector and, consequently, must be expressed in the form of a linear combination of the vectors $\nabla \tau_0$ and $\nabla \tau_1$, which merely define selected directions in the system. The second quantity, which describes the mean heat transfer between phases, must go to zero under steady-state conditions where $\tau_0 = \tau_1$. Considering further that both these quantities are proportional to the concentration of the dispersed phase, we then obtain the relations

$$\langle (1-\theta) \nabla T \rangle = \rho \mathbf{F}(\nabla \tau_0, \nabla \tau_1), \quad \langle (1-\theta) \nabla \mathbf{Q} \rangle = \rho \Phi(\tau_0, \tau_1), \quad (16)$$

where \mathbf{F} and Φ are certain previously unknown functionals which are linear with respect to their arguments. The hypothesis leading to the closure of the test-particle problem consists of an assumption that the conditional means $\langle (1-\theta) \nabla T \rangle^*$ and $\langle (1-\theta) \nabla \mathbf{Q} \rangle^*$ are expressed through τ_0^* , τ_1^* , and the volumetric concentration ρ^* of the dispersed phase in the neighborhood of the test particle by means of the same functionals \mathbf{F} and Φ , i.e.,

$$\langle (1-\theta) \nabla T \rangle^* = \rho^* \mathbf{F}(\nabla \tau_0^*, \nabla \tau_1^*), \quad \langle (1-\theta) \nabla \mathbf{Q} \rangle^* = \rho^* \Phi(\tau_0^*, \tau_1^*). \quad (17)$$

The actual solution of the test-particle problem which is closed by Eqs. (17) and the a posteriori determination of the form of these functionals from a comparison of Eqs. (16) and (14) is extremely laborious in the general case but can be carried out in various particular situations. An example of the solution of this problem under steady-state conditions for a medium with an arbitrary particle concentration as well as a study of the nonsteady-state problem for dilute dispersed media will be discussed in subsequent papers.

NOTATION

N , configuration of a system of N particles; a , particle radius; C, c , heat capacities per unit volume; \mathbf{F} , functional in Eqs. (16) and (17); G, g , arbitrary detailed function and its mean; H, h , intensities of internal heat sources; L, l , macroscopic and microscopic linear scales; N , total number of particles; n , calculated particle concentration; \mathbf{n} , unit normal vector; \mathbf{Q}, \mathbf{q} , thermal fluxes; $\mathbf{r}^{(i)}$, radius vector of the center of the i -th particle; T , local temperature; \mathbf{V}, \mathbf{v} , local and mean velocities; ε , volumetric concentration of continuous phase; η , Heaviside function; θ , structure function; Λ, λ , thermal conductivities; ξ , variable in Eq. (9); ρ , volumetric concentration of dispersed phase; σ , function in Eq. (9); τ , mean temperature; Φ , functional in Eqs. (16) and (17); φ , distribution function. Indices: 0, 1, continuous and dispersed phases, respectively; asterisk, conditional means.

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