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Heat and mass transfer in disperse media—I. Averaged field equations

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Abstract—Many important results concerning effective transport properties in a disperse system, including those secured under rather uncommon conditions, can be obtained with the help of the method of ensemble averaging combined with ideas of the self-consistent field theory. This justifies the undertaken careful consideration and partial revision of the basic ideas underlying both the method and the corresponding mathematical technique. An unequivocal set of conservation equations governing the transport of a scalar quantity in phases of the system on the average is also derived and formal representations for both the interphase exchange and the mean flux of the quantity in terms of integrals over the volume of some test particle are presented in the first part of the paper.

1. INTRODUCTION

AN EXHAUSTIVE description of all kinds of transport processes taking place in composite materials or in a dispersed heterogeneous media consisting of discrete inclusions (or particles) and an embedding continuous matrix is an old and important problem the complete solution of which is still far from being found. To a great extent, this is accounted for by the fact that the problem requires many complex, essentially different questions to be answered simultaneously. Among these, mention should be made of the questions pertaining to 'microscopic' features of the transport processes on the level of an individual inclusion and to collective interaction of many inclusions resulting in their joint influence on the observed 'macroscopic' transport properties. Proper statements of corresponding physical and mathematical problems, typical difficulties arising in attempts at their solution as well as the present state of the art on the whole and certain important advances are to be found in the review paper by Batchelor [1].

The global problem simplifies considerably when the macroscopic linear scale characterizing the mean parameters of a medium and the averaged field related to a physical quantity being transferred, substantially exceeds the microscopic scale associated with the internal structure of the medium and bearing upon the size and relative positions of inclusions. In such a case the macroscopic transport properties coincide with the bulk properties giving account of the general ability of the medium to transfer some conservable scalar or vector quantity, such as heat, mass, electric charge, momentum, and so forth. Then it seems quite natural to use continual methods for the overall description of transport processes regarding them as occurring in certain fictitious homogeneous continua which represent phases or components of the original medium. Within the scope of the theory of such co-existing continua two separate objectives of fundamental nature arise. The first consists in rigorous derivation of universal conservation equations that govern the transfer of heat, mass or another conservable quantity in each continuum, with the exchange of this quantity between the continua being allowed for. The second objective concerns the closure of the equations and amounts to the derivation of constitutive relations for all the unknown terms appearing in the conservation equations. Calculation of the bulk transport properties as functions of the physical and structural parameters of the medium is part of the latter problem.

The conservation equations are usually formulated by either using a postulative approach on the basis of purely phenomenological and semi-empirical reasoning or averaging local transport equations, valid inside homogeneous materials of both the matrix and the inclusions, over a representative time interval or a physically small volume of the mixture containing many inclusions. Refined versions of such a treatment are exemplified by refs. [2–7]. On the contrary, methods of quite different origin are usually employed for solving the closure problem. They have practically nothing in common with the methods of time or space averaging, utilized to obtain the conservation equations. It has become clear in recent years, that the effective solution of both problems is possible within the framework of a unified general approach based on the best use of the ensemble averaging technique together with some method specific for the self-consistent field theory.

The idea of averaging over a configurational ensemble of particles immersed into a continuous matrix seems to be first used in this context by Batchelor [8] in connection with the analysis of the rheological problem for dilute suspensions of rigid particles. Since then this idea has been extensively developed and applied to the description of other

NOMENCLATURE

a	radius of spheres
c	heat capacity per unit volume
D	diffusivity
j	density of inner heat sources
G, g	arbitrary fine-grained function and its average value
G', G^*	fluctuations of G
L, l	macro- and microscopic linear scales
N	total number of particles
n	number concentration of particles
$\mathbf{r}^{(j)}$	position vector of the jth sphere centre
$\mathbf{q}$	heat flux
$\mathbf{v}$	velocity.

Greek symbols

ε	porosity
θ	characteristic generalized function
λ	heat conductivity
ρ	concentration of particles by volume
τ	temperature
ϕ	probability distribution function.

Subscripts

0	ambient matrix
1	dispersed phase.

transport processes in mixtures of different concentrations. A review of the ensemble averaging technique and some aspects of the self-consistent field approximation, when applied to suspension flows is now available [9, 10].

The use of ensemble averaging has significant advantages over the time and space averaging. The derivation of the conservation equations and their closure, that is, the formulation of the constitutive relations, may be carried out by the same methods, so that there is no need to resort to supplementary models in order to obtain bulk transport properties. There is also no need for additional hypotheses about the possible connections between volume averages and corresponding quantities obtained by averaging over the other space objects (e.g. over planes differently oriented in space). By using the ensemble averaging one succeeds in formulating the bulk conservation equations in an entirely unambiguous form and, thus, in avoiding the latter problem the significance of which has been fairly pointed out in ref. [11]. It should also be mentioned that ensemble averaging leads to results which have an evident meaning in terms of the probability theory, and there is no necessity to require the presence of a great number of particles in physically small volumes of a disperse mixture as is the case for volume averaging. At last, a feasible way of generalization of all results and conclusions, obtained in comparatively simple situations peculiar to stationary transport in inactive media, to more complex situations is quite straightforward, so that there is no need to devise new special means in order to treat transport processes under unsteady conditions or in active media containing distributed sources or sinks of quantities partaking in these processes.

The general method under discussion has been virtually worked out in the last two decades and has been applied recently to a number of problems unapproachable by other means. Among these problems are the determination of the effective diffusivity of an admixture and of the effective thermal conductivity in a disperse medium characterized by internal heat and mass release [12], by appreciable contacts between neighbouring particles [13] and by chemical reactions and phase transitions at the particle surfaces [14] as well as to the investigation of dispersion effects accompanying unsteady transport processes [15]. Despite the adequacy of the method for solving nonstandard problems, it has never been set forth in a reasonably concise form. The intended purpose of this paper is, accordingly, to fill the gap as regards the formulation of both conservation and constitutive equations for heat or mass transfer.

The layout of the article is as follows. After giving an account of the mathematical formalism for dealing with the ensemble averaging procedure, which is the basis of the whole subsequent reasoning, the averaged field equations governing heat and mass transfer in the phases of a disperse mixture are derived in this first part of the article. Modifications of these equations valid in the vicinity of a chosen test particle of the mixture as well as the solution of the closure problem are studied in the second part of the paper.

2. ENSEMBLE AVERAGING

The development of an adequate mathematical formalism ensures a necessary foundation for averaging local transfer equations valid in the phases of a mixture. It provides a proper statistical smoothing and eliminates excessive details related to exact positions and orientations of all the particles as well as to local patterns of temperature and concentration fields in their vicinity. Then one is free to confine oneself to treating only a few observable quantities relevalent to the averaged picture of transport processes. Such a procedure of smoothing is not only convenient on the pragmatic ground but also appears to be perfectly natural. Really, mixtures differing in the types of particles and their packing can, nevertheless, correspond to the same macroscopic picture

and exhibit the same effective transfer properties. Besides, random parameters characterizing the mixture structure at the particle level are actually unknown. It seems obvious that the most general and consistent way of averaging has to include the concept of possible states of the system of particles.

To simplify the matter and to leave main ideas unencumbered by insignificant particulars, attention is given in what follows to a mixture consisting of N identical spherical particles immersed into a continuous matrix, both the particles and the matrix being separately homogeneous. It is assumed further that the motion of the particles relative to the matrix is either absent or sufficiently slow to prevent a notable influence of various convective effects on heat and mass transfer. That such an influence can be of importance is demonstrated in ref. [16]. This amounts to an assumption that the effective thermal and diffusive Peclet numbers for a single sphere are small as compared with unity. The sphere radius, a, and the structural microscopic length, l, characteristic of the particle arrangement are taken large compared with the molecular dimension so that the particles and the matrix can be viewed upon as continua. At the same time, these microscales are usually small as compared with the scale length, L, of essential changes in macroscopic properties of the mixture and in the fields of the mean temperature or admixture concentration.

2.1. *Ensemble distribution functions*

Any state of the dispersed phase of mixtures with identical spherical particles is completely characterized by a set of instantaneous position vectors, $\mathbf{r}^{(j)}$, $j = 1, \ldots, N$, of the centres of all the spheres and by sets of their time derivatives of different order. In as much as the relative motion of the mixture phases is taken to be negligible, it becomes possible to exclude the time derivatives and to make allowance only for the position vectors. Then, the states which correspond to the same collection of position vectors but to different sets of particle velocities, accelerations, etc. have to be regarded as indistinguishable. A rigorous substantiation of such an idea for disperse systems with moving phases is presented in ref. [17] where the conservation equations have been proved (with the help of Feynman's technique of integrals over random trajectories), to preserve their form when each position vector is thought of as a function of time with possible discontinuities modelling collisions between the particles. Thus, one arrives at a concept of the configurational ensemble of the assemblage of particles. Members of the ensemble are symbolized by discernable sets of the vectors $\mathbf{r}^{(j)}$ acceptable from a physical point of view.

In a more general case, when the particles are of the same but arbitrary form and of different size, it is necessary to incorporate into the analysis two complementary sets of unit orientation vectors locked inside each particle and to introduce likewise a linear scale of the particles as a new independent ensemble variable.

The properties of the configurational ensemble of equal spheres can be determined to the full if a distribution function, $\phi(C_N)$, is given. Here C_N is the configurational phase space for the whole of the assemblage generated by N vectors $\mathbf{r}^{(j)}$ with due regard for the inequalities $|\mathbf{r}^{(i)} - \mathbf{r}^{(j)}| \geqslant 2a$, $i \neq j$, which result from the condition of non-overlapping of the hard spheres. Exclusive cases of strictly ordered systems, the particles of which are positioned in a prescribed manner so that their centres occupy the points of some regular lattice, can be included into the analysis by allowing for the ensemble distribution function to be expressed in terms of proper delta-functions.

Along with $\phi(C_N)$, one is able to introduce conditional distribution functions $\phi(C_{N-1}|\mathbf{r})$, $\phi(C_{N-2}|\mathbf{r}, \mathbf{r}')$, ... pertaining to the configurational ensembles of $N-1$, $N-2$, ... spheres, the positions of one, two or more spheres being fixed. Presuming that all the distribution functions are normalized to unity one can come, by integrating over the position vectors of a number of particles, to unconditional or conditional distribution functions for the remaining particles. Especially important are the distribution functions $\phi(\mathbf{r})$ and $\phi(\mathbf{r}, \mathbf{r}')$ for one and two spheres derived after integrating $\phi(C_N)$ over the position vectors of the other spheres,

$$\phi(\mathbf{r}, \mathbf{r}') = \int \phi(C_N) \prod_{j=1, j\neq i,k}^{N} \mathrm{d}\mathbf{r}^{(j)}|_{\mathbf{r}^{(i)}=\mathbf{r}, \mathbf{r}^{(k)}=\mathbf{r}'}$$

$$\phi(\mathbf{r}) = \int \phi(\mathbf{r}, \mathbf{r}')\, \mathrm{d}\mathbf{r}'. \tag{1}$$

The latter function can be regarded as the unconditional probability density of a single particle centre being located at the point $\mathbf{r}$, the former one defines the probability density of this event conditioned by the presence of another sphere centre at the point $\mathbf{r}'$. Obviously,

$$\phi(C_N) = \phi(\mathbf{r})\phi(C_{N-1}|\mathbf{r}),$$

$$\phi(C_{N-1}|\mathbf{r}) = \phi(\mathbf{r}, \mathbf{r}')\phi(C_{N-2}|\mathbf{r}, \mathbf{r}'), \ldots. \tag{2}$$

Note that for the sake of simplicity the time, t, is omitted from the arguments of the distribution functions. This fits mixtures with permanent relative positioning of particles, such as granular composite materials and fixed particulate beds.

2.2. *Ensemble averages*

Let $G(t, \mathbf{r}|C_N)$ be a 'fine-grained' function of time and coordinates characterizing some physical quantity and depending in addition on the arrangement of particles. This function must be a generalized one, that is, it is well defined inside both the matrix and the particles where it is continuous but may have discontinuities at interfaces. The ensemble unconditioned average of $G(t, \mathbf{r}|C_N)$ is to be defined as

$$g(t,\mathbf{r}) = \langle G\rangle = \int G(t,\mathbf{r}|C_N)\phi(C_N)\,\mathrm{d}C_N. \quad (3)$$

Conditional averages have to be defined in a similar way. For example,

$$g(t,\mathbf{r}|\mathbf{r}') = \langle G\rangle_{\mathbf{r}'} = \int G(t,\mathbf{r}|C_N)\phi(C_{N-1}|\mathbf{r}')\,\mathrm{d}C_{N-1} \quad (4)$$

is calculated by integrating over all physically permissible values of $\mathbf{r}^{(j)}$, $j = 1,\ldots,N-1$, compatible with the condition that the centre of one of the spheres lies at the point $\mathbf{r}'$. It follows from equations (1) to (4) that

$$g(t,\mathbf{r}) = \int g(t,\mathbf{r}|\mathbf{r}')\phi(\mathbf{r}')\,\mathrm{d}\mathbf{r}',$$

$$g(t,\mathbf{r}|\mathbf{r}') = \int g(t,\mathbf{r}|\mathbf{r}',\mathbf{r}'')\,\phi(\mathbf{r}',\mathbf{r}'')\,\mathrm{d}\mathbf{r}'',\ldots. \quad (5)$$

Apart from equations (3) and (4), which define the averages attributed to the mixture as a whole, it is also possible to determine averages associated with the mixture phases. For this purpose it is convenient to put forward the detailed density of centres of the spheres, that is,

$$N(\mathbf{r}|C_N) = \sum_{j=1}^{N}\delta(\mathbf{r}-\mathbf{r}^{(j)}) \quad (6)$$

and the characteristic function

$$\theta(\mathbf{r}|C_N) = 1-\sum_{j=1}^{N}H(a-|\mathbf{r}-\mathbf{r}^{(j)}|) \quad (7)$$

which assumes zero value at points within the particles and equals unity in the interstices, $\delta(x)$ and $H(x)$ being the Dirac delta-function and the Heaviside step function, respectively.

Equations (6) and (7) enables one to determine the mean number concentration of particles and their mean concentration by volume, that is,

$$n(\mathbf{r}) = \langle N(\mathbf{r}|C_N)\rangle = N\langle\delta(\mathbf{r}-\mathbf{r}^{(j)})\rangle = N\phi(\mathbf{r}),$$

$$\rho(\mathbf{r}) = 1-\langle\theta\rangle = N\langle H(a-|\mathbf{r}-\mathbf{r}^{(j)}|)\rangle$$

$$= \int_{|\mathbf{r}-\mathbf{r}'|\leqslant a} n(\mathbf{r}')\,\mathrm{d}\mathbf{r}'. \quad (8)$$

In particular, neglecting the terms of the order a/L, if such an action is permissible, one obtains from equation (8) a familiar relation

$$\rho(\mathbf{r}) = \tfrac{4}{3}\pi a^3 n(\mathbf{r}). \quad (9)$$

Similarly, conditional averages corresponding to equation (8) are to be written as

$$n(\mathbf{r}|\mathbf{r}') = N\langle\delta(\mathbf{r}-\mathbf{r}^{(j)})\rangle_{\mathbf{r}'} = N\phi(\mathbf{r},\mathbf{r}'),$$

$$\rho(\mathbf{r}|\mathbf{r}') = N\langle H(a-|\mathbf{r}-\mathbf{r}^{(j)}|)\rangle_{\mathbf{r}'}$$

$$= \int_{|\mathbf{r}-\mathbf{r}'|\leqslant a,\,|\mathbf{r}'-\mathbf{r}''|>2a} n(\mathbf{r}''|\mathbf{r}')\,\mathrm{d}\mathbf{r}''. \quad (10)$$

Here the inequality $N \gg 1$ is taken into account. Both unconditional and conditional matrix concentrations by volume are to be brought into action along with those for the particles

$$\varepsilon(\mathbf{r}) = 1-\rho(\mathbf{r}),\quad \varepsilon(\mathbf{r}|\mathbf{r}') = 1-\rho(\mathbf{r}|\mathbf{r}'). \quad (11)$$

It is worthwhile noting that while the linear scale of $\rho(\mathbf{r})$ and $\varepsilon(\mathbf{r})$ equals L by definition the scale of the corresponding conditional quantities in equation (11) is of the order of a.

Now the unconditional phase averages bearing separately upon the matrix and the particles are to be defined as

$$\varepsilon(\mathbf{r})g_0(t,\mathbf{r}) = \langle\theta G\rangle = \int\theta G(t,\mathbf{r}|C_N)\phi(C_N)\,\mathrm{d}C_N,$$

$$\rho(\mathbf{r})g_1(t,\mathbf{r}) = \langle(1-\theta)G\rangle$$

$$= \int(1-\theta)G(t,\mathbf{r}|C_N)\phi(C_N)\,\mathrm{d}C_N \quad (12)$$

where the subscripts 0 and 1 refer henceforth to the matrix and the particles, respectively. Similar expressions can be written for averages conditioned by the presence of the sphere centre at the point $\mathbf{r}'$. Namely,

$$\varepsilon(\mathbf{r}|\mathbf{r}')g_0(t,\mathbf{r}|\mathbf{r}') = \langle\theta G\rangle_{\mathbf{r}'}$$

$$= \int\theta G(t,\mathbf{r}|C_N)\phi(C_{N-1}|\mathbf{r}')\,\mathrm{d}C_{N-1},$$

$$\rho(\mathbf{r}|\mathbf{r}')g_1(t,\mathbf{r}|\mathbf{r}') = \langle(1-\theta)G\rangle_{\mathbf{r}'}$$

$$= \int(1-\theta)G(t,\mathbf{r}|C_N)\phi(C_{N-1}|\mathbf{r}')\,\mathrm{d}C_{N-1}. \quad (13)$$

Relations similar to those in equation (5) follow from equations (2), (12) and (13). The definition of the averages in equations (3), (4) and (12) leads to the equations

$$g(t,\mathbf{r}) = \varepsilon(\mathbf{r})g_0(t,\mathbf{r})+\rho(\mathbf{r})g_1(t,\mathbf{r}),$$

$$g(t,\mathbf{r}|\mathbf{r}') = \varepsilon(\mathbf{r}|\mathbf{r}')g_0(t,\mathbf{r}|\mathbf{r}')+\rho(\mathbf{r}|\mathbf{r}')g_1(t,\mathbf{r}|\mathbf{r}'). \quad (14)$$

The expressions for the averages over the dispersed phase can be reduced to a form analogous to that of the last formulae in equations (8) and (10). By using the definition of θ in equation (7) one gets

$$\rho(\mathbf{r})g_1(t,\mathbf{r}) = \int_{|\mathbf{r}-\mathbf{r}'|\leqslant a} n(\mathbf{r}')g_1(t,\mathbf{r}|\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

$$= n(\mathbf{r})\int_{x\leqslant a} g_1(t,\mathbf{r}+\mathbf{x}|\mathbf{r})\,\mathrm{d}\mathbf{x}+0\left(\frac{a}{L}\right),$$

$$\rho(\mathbf{r}|\mathbf{r}')g_1(t,\mathbf{r}|\mathbf{r}') = \int_{|\mathbf{r}-\mathbf{r}'|\leqslant a,\,|\mathbf{r}'-\mathbf{r}''|>2a} n(\mathbf{r}''|\mathbf{r}')g_1(t,\mathbf{r}|\mathbf{r}',\mathbf{r}'')\,d\mathbf{r}''. \quad (15)$$

As before, one here takes advantage of the fact that the spheres are statistically undistinguishable. In the former relation the integration is carried out over those values of $\mathbf{r}'$ that the sphere of radius a, the centre of which lies at the point $\mathbf{r}'$, contains a given point $\mathbf{r}$. In the latter relation the role of the variable of integration is played by $\mathbf{r}''$ and the non-overlapping condition for the spheres of the same radius with the centres at $\mathbf{r}'$ and $\mathbf{r}''$ is imposed in addition. As far as the present author is aware, integrals of such a type were brought into practice for the first time in ref. [18].

Relations of the type of those numbered (15) can be written also for averages over the dispersed phase conditioned by prescribing positions of more than one particle. Then a conditional average, conforming to the requirement that the location of the centres of M spheres is given, has to be expressed as an integral of the corresponding average with $M+1$ sphere centres being fixed, multiplied by a suitable conditional number concentration of the particles. Thus, there is a practically infinite ($N \gg 1$) train of integral relations resembling those numbered (15) and connecting conditional averages over the dispersed phase. In this context a problem of closure or truncation of this train arises which will be explicitly considered later. Note that equations (15) play a fundamental role in what follows.

Owing to the independence of the distribution functions of the time and space variables, the operators of ensemble averaging commute with the differentiation with respect to both t and $\mathbf{r}$. For the unconditional averages one has

$$\langle \partial G/\partial t\rangle = \partial g(t,\mathbf{r})/\partial t, \quad \langle \partial G/\partial \mathbf{r}\rangle = \partial g(t,\mathbf{r})/\partial \mathbf{r}. \quad (16)$$

Similar equalities are valid for all the conditional averages in disperse systems with both motionless and moving particles.

2.3. *Fluctuations*

There are two alternative ways of introducing fluctuations of an arbitrary fine-grained function $G(t,\mathbf{r}|C_N)$ about its averaged value. 'Physical' fluctuations relative to the phase averages are to be determined by means of obvious relations

$$\theta G = \theta g_0 + \theta G',$$
$$(1-\theta)G = (1-\theta)g_1 + (1-\theta)G'. \quad (17)$$

It is clear that $G'(t,\mathbf{r}|C_N)$ represents a generalized function the exact definition of which is dictated by the physical meaning of $G(t,\mathbf{r}|C_N)$, and its values inside the particles may be essentially different from those within the interstices. It is quite evident that $\langle \theta G'\rangle = \langle (1-\theta)G'\rangle = \langle G'\rangle = 0$.

Besides, it is possible to introduce a fluctuating function $G^*(t,\mathbf{r}|C_N)$ with reference to deviations of $G(t,\mathbf{r}|C_N)$ from its mean value $g(t,\mathbf{r})$ associated with the disperse mixture as a whole when one does not know exactly whether the point $\mathbf{r}$ belongs to the particles or to the matrix. Thus, one assumes

$$G(t,\mathbf{r}|C_N) = g(t,\mathbf{r}) + G^*(t,\mathbf{r}|C_N). \quad (18)$$

It is quite simple to show that

$$\langle G\rangle_{\mathbf{r}'} = g(t,\mathbf{r}) + g^*(t,\mathbf{r}|\mathbf{r}'),$$
$$\langle \theta G\rangle_{\mathbf{r}'} = \varepsilon(t,\mathbf{r})g_0(t,\mathbf{r}) + \varepsilon(t,\mathbf{r}|\mathbf{r}')g_0^*(t,\mathbf{r}|\mathbf{r}')$$
$$\langle (1-\theta)G\rangle_{\mathbf{r}'} = \rho(t,\mathbf{r})g_1(t,\mathbf{r}) + \rho(t,\mathbf{r}|\mathbf{r}')g_1^*(t,\mathbf{r}|\mathbf{r}') \quad (19)$$

where the notations

$$g^*(t,\mathbf{r}|\mathbf{r}') = \langle G\rangle_{\mathbf{r}'}^*,$$
$$\varepsilon(t,\mathbf{r}|\mathbf{r}')g_0^*(t,\mathbf{r}|\mathbf{r}') = \langle \theta G^*\rangle_{\mathbf{r}'},$$
$$\rho(t,\mathbf{r}|\mathbf{r}')g_1^*(t,\mathbf{r}|\mathbf{r}') = \langle (1-\theta)G^*\rangle_{\mathbf{r}'} \quad (20)$$

are used. When $|\mathbf{r}-\mathbf{r}'| \to \infty$ all the averages marked with an asterisk go to zero.

In contrast to fluctuations of the type of $G'(t,\mathbf{r}|C_N)$, fluctuations of the type of $G^*(t,\mathbf{r}|C_N)$ have no immediate physical meaning or interpretation. This reflects, to a degree, an inherent lack of our knowledge of whether the variable vector $\mathbf{r}$ lies in the particles or in the interstices. However, the latter fluctuations happen to be very useful while attempting to describe in an explicit form perturbations induced to the fields $g(t,\mathbf{r})$, $g_0(t,\mathbf{r})$ and $g_1(t,\mathbf{r})$ by either a fixed sphere or a solid impenetrable wall bounding the mixture under study. They prove to be rather helpful in both solution of the closure problem and analysis of boundary effects.

3. AVERAGED TRANSPORT EQUATIONS

The main aim of the following analysis consists in rigorous derivation of conservation equations, which govern heat or mass transfer processes in a heterogeneous mixture on the macroscopic scale, by means of the ensemble averaging of local heat conduction or diffusion equations valid in the materials of the mixture phases. Below, for the sake of definiteness, the heat conduction is considered keeping in mind that all the results may be well applied without substantial changes to diffusion and some other processes.

Since the relative motion of the phases is assumed to be unimportant, it is reasonable to use a reference frame in which the mixture is motionless as a whole. Then the heat conduction equation in the materials of both phases can be presented as a single generalized equation

$$C\partial T/\partial t = -\nabla \mathbf{Q} + J, \quad \mathbf{Q} = -\Lambda(\partial T/\partial \mathbf{r}), \quad (21)$$

where T and $\mathbf{Q}$ are understood as generalized scalar

and vector functions describing in detail the temperature and heat flux in the mixture, respectively. Generalized functions C and Λ, representing the heat capacity per unit volume and the heat conductivity, as well as the function J, characterizing the intensity of possible inner heat sources, are to be expressed in the form

$$C = \theta c_0 + (1-\theta)c_1, \quad \Lambda = \theta\lambda_0 + (1-\theta)\lambda_1,$$
$$J = \theta j_0 + (1-\theta)j_1, \tag{22}$$

where c_i, λ_i and j_i are the specific heat capacities related to unit volume, the heat conductivities and the densities of heat sources in the materials of the matrix and of the particles.

By averaging over the ensemble distribution function $\phi(C_N)$ of relations resulting from the first equation in set (21) after multiplication by $1-\theta$ and θ, one obtains the following equations for the mean temperatures τ_0 and τ_1 of the mixture phases:

$$\varepsilon c_0(\partial\tau_0/\partial t) = -\partial\mathbf{q}/\partial\mathbf{r} + \langle(1-\theta)(\partial\mathbf{Q}/\partial\mathbf{r})\rangle + \varepsilon j_0,$$
$$\rho c_1(\partial\tau_1/\partial t) = -\langle(1-\theta)(\partial\mathbf{Q}/\partial\mathbf{r})\rangle + \rho j_1,$$
$$\tau_0(t,\mathbf{r}) = \langle\theta T\rangle, \quad \tau_1(t,\mathbf{r}) = \langle(1-\theta)T\rangle,$$
$$\mathbf{q}(t,\mathbf{r}) = \langle\mathbf{Q}\rangle, \quad j_0(t,\mathbf{r}) = \langle\theta J\rangle,$$
$$j_1(t,\mathbf{r}) = \langle(1-\theta)J\rangle. \tag{23}$$

The commutability equations (16), the identification of C and J in equations (22) and the obvious relation $\langle\theta\partial\mathbf{Q}/\partial\mathbf{r}\rangle = \nabla\langle\mathbf{Q}\rangle - \langle(1-\theta)(\partial\mathbf{Q}/\partial\mathbf{r})\rangle$ are used when deriving equations (23).

By summing up the equations in set (23) one gets

$$c\partial\tau/\partial t = -\partial q/\partial\mathbf{r} + j, \quad c = \varepsilon c_0 + \rho c_1, \quad j = \varepsilon j_0 + \rho j_1, \tag{24}$$

where τ is the mean mixture temperature expressed in terms of τ_0 and τ_1 in accordance with equation (14) and c, j are associated with the mixture as a whole. Thus, the averaged heat transfer equations are defined completely, if a link between the mean heat flux $\mathbf{q}$ and the mean phase temperatures τ_0 and τ_1 is established.

The averaging of the second equation in set (21) with the help of equations (16) and (22) leads to

$$\mathbf{q} = -\langle\Lambda\nabla T\rangle = -\lambda_0\langle\theta\nabla T\rangle - \lambda_1\langle(1-\theta)\nabla T\rangle$$
$$= -\lambda\nabla\tau - (\lambda_1-\lambda_0)\langle(1-\theta)\nabla T\rangle. \tag{25}$$

Regarding j_0 and j_1 as known quantities, it is seen that equations (23) and (24) contain only two unknown terms, $\langle(1-\theta)\nabla\mathbf{Q}\rangle$ and $\langle(1-\theta)\nabla T\rangle$, which both represent certain averages over the dispersed phase. The first term characterizes the heat exchange between the phases per unit volume of the mixture whereas the second one bears on a deviation of the mean heat flux in an actual disperse medium from that in a one-phase homogeneous continuum the heat conductivity of which happens to coincide with that of the matrix material. To make the unknown variables τ_0 and τ_1 determinable by solving equations (23), one needs to express the mentioned terms in an explicit form as functions of these variables and their derivatives. It is this procedure which constitutes the essence of the closure problem for the averaged heat transfer equations and the resulting expressions are to be looked upon as constitutive relations for the mixture under study.

The key idea underlying the closure problem involves expressing these unknown quantities through the use of relations (15) in the following manner:

$$\langle(1-\theta)\nabla\mathbf{Q}\rangle = \int_{|\mathbf{r}-\mathbf{r}'|\leqslant a} n(\mathbf{r}')\nabla_{\mathbf{r}}\mathbf{q}(t,\mathbf{r}|\mathbf{r}')\,\mathrm{d}\mathbf{r}',$$
$$\langle(1-\theta)\nabla T\rangle = \int_{|\mathbf{r}-\mathbf{r}'|\leqslant a} n(\mathbf{r}')\nabla_{\mathbf{r}}\tau(t,\mathbf{r}|\mathbf{r}')\,\mathrm{d}\mathbf{r}'. \tag{26}$$

So far, use has been made of the reference frame connected with the mean motion of the mixture on the whole. Generalization to more complicated situations when both phases are moving is straightforward and leads to equations

$$\varepsilon c_0(\partial/\partial t + \mathbf{v}_0\nabla)\tau_0 = -\partial\mathbf{q}/\partial\mathbf{r} + \langle(1-\theta)(\partial\mathbf{Q}/\partial\mathbf{r})\rangle + \varepsilon j_0,$$
$$\rho c_1(\partial/\partial t + \mathbf{v}_1\nabla)\tau_1 = -\langle(1-\theta)(\partial\mathbf{Q}/\partial\mathbf{r})\rangle + \rho j_1 \tag{27}$$

written in the laboratory coordinate system. They have to be substituted for those in set (23). Here $\mathbf{v}_0$ and $\mathbf{v}_1$ are the mean velocities of the ambient matrix within the interstices and of the particles, respectively. Formulae (26) remain true under the imposed assumption that the Peclet number for a single particle is much smaller than unity to assure negligibility of the influence of a relative flow on the heat transfer either to or from the particle surface. This means, in particular, that the relative velocity $\mathbf{v}_0 - \mathbf{v}_1$ must be sufficiently small as well [16].

All the results are valid for the processes of diffusion of an admixture in a disperse medium if C is substituted by unity and the thermal conductivities λ_0 and λ_1 are replaced by the diffusivities D_0 and D_1. Then τ_0 and τ_1 play roles of the mean concentrations of the admixture in the matrix and in the particles, respectively.

Note that the discrete nature of the dispersed phase is evidently taken into account while formulating all the equations presented above. This means the effect of possible direct contacts between particles to be set aside and, therefore, a component of the total heat flux due to transport through permanent or instantaneous contact areas of touching or colliding particles to be overlooked.

4. CONCLUDING REMARKS

The averaged field equations derived above for heat and mass transfer in disperse media are principally of the same form as those obtained with the help of other approaches (see, for example, refs. [2–7]). However, the very procedure of their derivation is not only of some methodological interest but also throws light

on the possible methods for managing the closure problem. It follows from equations (26) that the unknown variable terms involved in equations (23) and (27) could be found by means of simple integration, if one would be successful in determining explicit representations for the quantities $q(t, \mathbf{r}|\mathbf{r}')$ and $\tau(t, \mathbf{r}|\mathbf{r}')$ conditioned by the presence of a test sphere centre at the point $\mathbf{r}'$. When $|\mathbf{r}-\mathbf{r}'| \leqslant a$, these quantities represent the mean heat flux and the temperature inside the test sphere obtained by averaging over the ensemble of allowable configurations of all the other spheres, that is, over the conditional ensemble distribution function. Equations governing heat transfer around the test sphere on the average can be derived by employing methods quite similar to those used above. In such a way, the necessary link between the macroscopic continual description of heat conduction and the study of heat transfer processes on the microscopic level of individual particles is ensured.

Various ways of calculating equations (26) and, thereby, of solving the closure problem will be considered in detail in the second part of this paper.

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TRANSFERT DE CHALEUR ET DE MASSE DANS LES MILIEUX DISPERSES—I. EQUATIONS DE CHAMP MOYENNEES

Résumé—Des résultats importants concernant les propriétés effectives de transport dans un système dispersé, incluant ceux relatifs à des conditions plutôt rares, peuvent être obtenus par une méthode de moyenne d'ensemble combinée aux idées de la théorie de champ auto-cohérent. Cela justifie l'examen soigneux et la révision partielle des idées de base concernant à la fois la méthode et la technique mathématique correspondante. Un système d'équations de conservation gouvernant le transport d'une grandeur scalaire dans une phase du système est obtenu et des représentations formelles pour l'échange interphase et le flux moyen de la grandeur en fonction des intégrales sur le volume est présenté dans la première partie de cette étude.

WÄRME- UND STOFFTRANSPORT IN DISPERSEN MEDIEN—I. GEMITTELTE FELDGLEICHUNGEN

Zusammenfassung—Viele wichtige Ergebnisse im Hinblick auf die effektiven Transportvorgänge in einem dispersen System, auch solche die unter ziemlich ungewöhnlichen Bedingungen auftreten, können mit Hilfe des Verfahrens der Ensemble-Mittelung in Kombination mit den Vorstellungen der selbstkonsistenten Feldtheorie ermittelt werden. Dies rechtfertigt die unternommene sorgfältige Betrachtung und teilweise Revision der Vorstellung, die dem Verfahren und der entsprechenden mathematischen Behandlung zugrunde liegt. Es wird ein eindeutiger Satz von Erhaltungsgleichungen für den Transport einer Skalargröße in einer Phase des gemittelten Systems abgeleitet. Außerdem wird im ersten Teil der Arbeit eine formale Beschreibung für den Austausch zwischen den Phasen und die mittlere Stromdichte der Größe als Integralterm über das Volumen einiger Testpartikel vorgestellt.

ТЕПЛО- И МАССОПЕРЕНОС В ДИСПЕРСНЫХ СРЕДАХ.—I. УСРЕДНЕННЫЕ УРАВНЕНИЯ ПОЛЯ

Аннотация—Многие важные результаты по эффективным характеристикам переноса в дисперсной системе, в том числе и в несколько необычных условиях, можно получить при помощи метода ансамблевого усреднения в сочетании с идеями теории самосогласованного поля. Это оправдывает предпринятые ниже подробный анагиз и частичный пересмотр основных положений как самого метода, так и соответствующего математического аппарата. В первой жасти работы сформулирована вполне определенная система уравнений сохранения, определяющая в среднем перенос скалярной величины в фазах дисперсной среды, и представлены формальные выражения для межфазового обмена и среднего потока этой величины через интегралы по объему некоторой пробной частицы.