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SOME PARTICULAR CASES OF THE TWO-DIMENSIONAL INTEGRODIFFERENTIAL EQUATION OF PARTICLE TRANSFER

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Some particlar cases are derived from the integrodifferential equation of particle transfer with a constant rate: they are the diffusion approximation and a differential equation of diffusion (heat conduction) of hyperbolic type with a finite velocity of propagation of perturbations.

1. Introduction. In description of some heat and mass transfer phenomena, it should be taken into consideration that heat (mass) propagates through a continuum with a finite velocity. This leads to the necessity of generalization of conventional heat-conduction and diffusion equations based on Fourier's and Fick's laws and resulting in an infinite velocity of propagation of perturbations. A phenomenological description of heat and mass transfer with a finite rate was considered, in particular, in [1, 2]. Some equations are suggested in [3, 4] for description of substance transfer with a finite rate on the basis of a certain theoretical scheme at the microlevel.

In what follows we derive some particular cases from Tolubinskii's kinetic equation [3, 4], having obtained, in particular, transfer equations of diffusion type from it. Until now, this equation has not been widely used, although some useful results obtained on its basis have been pointed out [5]. In this equation we are attracted by the fact that in the general case it can be used for analysis of transfer processes in a continuum with variable properties at a finite velocity of propagation of perturbations. Repeated attempts (for example, [6-8]) to derive the wave equation of heat conduction (diffusion) were effective only in the one-dimensional case in the space coordinate, and therefore the equation given in [3, 4] and some of particular cases of it in the literature [2, 9] are considered as a basis for derivation (analysis) of the heat-conduction equation with a finite velocity of propagation of perturbations. These equations are now of interest both for description of some problems of propagation of running waves of combustion type (nerve fibers etc. [10]) and for analysis of processes occurring in chemical reactors, where under certain conditions it is necessary to reject the conventional diffusion model [11, 12]. It should also be noted that some attempts are made [13, 14] to justify "wave equations" of diffusion in the non-one-dimensional case on the basis of other approaches (for example, from Boltzmann's equation [14]). These approaches also contain certain hypotheses and assumptions.

In the simplest case, in derivation of the integrodifferential transfer equation [4], it is assumed that transfer or diffusion of mass can be considered as random wandering with a constant velocity C of the particles of the substance or the carriers of energy in a medium whose properties are specified by the functions $\mu(P, T)$ and Φ(u, v, P, T). The first function $\mu(P, T)$ is the probability density of interaction (collision) of the particles at the time T with elements of the medium at the point P determined by the coordinates X, Y in the two-dimensional case and X, Y, Z in the three-dimensional case. The second function Φ is the probability density of a change in the direction of motion of a particle from u to v because of collision with an element at the point P. In the two-dimensional case (and here we restrict ourselves to it) the direction is characterized by one angle, and, therefore, the function $\Phi(\varphi, \psi, P, T)$ has written-out arguments. As a probability density this function is nonnegative and satisfies the following conditions:

$$\int_{-\pi}^{\pi} \Phi(\varphi, \psi, X, Y, T)\, d\psi = \int_{-\pi}^{\pi} \Phi(\varphi, \psi, X, Y, T)\, d\varphi = 1\,, \tag{1}$$

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where the first of the equalities expresses the fact that after interaction with the medium a particle has some direction of motion ψ in the range of angles $\psi \in (-\pi, \pi)$ with certain probability. The second equality in (1) is a limitation that we imposed on the function Φ. Together with other conditions for Φ (see below, Sec. 2), this equality makes some calculations single-valued. In particular, the effect of this equality consists in the fact that it eliminates terms connected with "scatter" of particles in transfer equation (3) given below and integrated over φ between $(-\pi)$ and (π), i.e., this equality corresponds to a certain "law of conservation" in interaction of particles with the medium. This statement is consistent with the adopted model of interaction that occurs without energy exchange [4], i.e., the effect of the medium is exhibited only in a change in the direction of motion of the particles but not in the absolute value of its velocity. It should also be noted that the function $\mu(P, T)$ is the inverse of the mean free path of a particle [4], i.e, it is connected with the density of the medium.

For the kinetic equation of [4] the main unknown function is the conventional probability H of transition of a particle from the point $Q(\xi, \eta)$, found there at the time τ, to the point $P(X, Y)$ correspondingly at the time T $(T > \tau)$ as the direction of motion changes from u to v, i.e., in the two-dimensional case we have $H(Q, \tau, \psi, P, T, \varphi)$. In accordance with [4], the function H written in terms of the arguments results from a certain integration that includes the conventional probability density $f(P)$ that at the time τ the particle occurs at the point P of the space $(\tau < T)$ and the conventional probability density $J(P, \mathrm{v})$ that at the time τ the particle leaves the point P. Here, the function H^* corresponding to the initial data $f = \delta(Q - P)$ and $J = \delta(\mathrm{u} - \mathrm{v})$, where $\delta(z)$ is the Dirac delta-function, plays the main role. Thus, we have

$$H = \int\limits_R f(Q)\, d\xi d\eta \int\limits_{-\pi}^{\pi} J(Q, \omega)\, H^*(Q, \tau, \omega, P, T, \varphi)\, d\omega\,, \tag{2}$$

where R is the region of two-dimensional space of interest. According to (2), H is a functional of f and J, the arguments of H written above are exact only for the function H^*; however, we retain the previous notation since the first three arguments will be parametric in the sequel and, whenever necessary, it may be assumed that the relations considered were already subjected to integration similar to (2).

In monograph [4] some natural generalizations of the described probability model and the relation of the functions μ and Φ (i.e., their actual definition) with concrete physical parameters (thermal conductivity of metals, two-component diffusion, etc.) are discussed. Here, we concentrate our attention on the above-defined statements without concrete physical applications, and for definiteness the obtained equations will be called diffusion equations, although their application is far from being restricted to diffusion processes proper [4]. It should also be noted that transfer equations similar to or coinciding in form with Tolubinskii's equation are used for analysis of neutron transfer in a substance, thermal radiation, diffusion of a light gas in a heavy one, and, probably, some other processes similar in physical and mathematical aspects [15-17].

In technological equipment, conditions of mass transfer change noticeably in various parts of it, depending on its design, operating conditions, etc. This leads to diverse theoretical schemes of description of transfer processes in such equipment (various modifications of diffusion and cellular models, account for stagnation areas, bypass flows, etc.) [18, 19]. In this situation, the approach of [3, 4] allows a new look at the processes in the equipment, specifying its characteristics μ and Φ in parts of the space with specific conditions of substance transfer. In this case the equations of [3, 4] function as microequations for the models of [18, 19] and extend these models to cases of propagation of mass (heat) with a finite velocity. Here we restrict ourselves to consideration of Tolubinskii's two-dimensional (in the coordinates) equation, from which we obtain the diffusion approximation and a diffusion equation of hyperbolic type.

2. Derivation of the Diffusion Equation. According to [4], the basic kinetic equation for determination of the function H has the form

$$\frac{\partial H}{\partial T} + C\left(\cos(\varphi)\frac{\partial H}{\partial X} + \sin(\varphi)\frac{\partial H}{\partial Y}\right) + C\mu(P, T)\, H(Q, \tau, \psi, P, T, \varphi) =$$

$$= C\mu (P, T) \int_{-\pi}^{\pi} \Phi (\beta, \varphi, P, T) H (Q, \tau, \psi, P, T, \beta) d\beta , \tag{3}$$

where C is the particle velocity. Below, whenever it does not bring about confusion, some or all of the arguments of the functions Φ and H are omitted. The following dimensionless coordinates and parameters are introduced:

$$x = X/L , \quad y = Y/L , \quad t = C\lambda T/L^2 , \quad \nu (P, t) = \mu\lambda , \quad \varepsilon = \lambda/L , \tag{4}$$

where L is the characteristic length of the region of noticeable variation of the function H; λ is the scale of the mean free path of a particle, equal in magnitude [4] to the inverse of the scale of the function μ. Thus, relation (3) is rewritten as

$$\varepsilon^2 \frac{\partial H}{\partial t} + \varepsilon \left(\cos (\varphi) \frac{\partial H}{\partial x} + \sin (\varphi) \frac{\partial H}{\partial y}\right) + \nu (P, t) H (\dots , P, t, \varphi) =$$

$$= \nu (P, t) \int_{-\pi}^{\pi} \Phi (\beta, \varphi, P, t) H (\dots , P, t, \beta) d\beta . \tag{5}$$

Assuming the parameter ε to be a small quantity, i.e., $\lambda << L$, we consider a typical situation for continua. The time scale $L^2/C\lambda$ is chosen rather large, which also appears in analysis of transfer macroproblems. Here, our objective is to obtain a simpler (conventional) diffusion equation in the limiting case $\varepsilon \to 0$ from (5). To do this, it is natural to use the method of a small parameter [20, 21].

The solution of Eq. (5) is sought in the form of the series

$$H = H_0 + \varepsilon H_1 + \varepsilon^2 H_2 + \dots , \tag{6}$$

after substitution of (6) into (5) and retention of terms of the same order of magnitude with respect to ε we obtain in the principal approximation the expression

$$H_0 (\dots , P, t, \varphi) = \int_{-\pi}^{\pi} \Phi (\beta, \varphi, P, t) H_0 (\dots , P, t, \beta) d\beta . \tag{7}$$

It can easily be seen that because of (1), this formula is satisfied by the function $H_0 = G(P, t)$, where the first arguments are omitted. This indicates that the set of eigenfunctions of Eq. (7) is not empty. In the general case the number of eigenfunctions of this expression depends on the kernel Φ. In particular, for $\Phi = \delta(\varphi - \beta)$ any function H_0 satisfies (7). This variant is of little interest since it is the case of no "scatter" of particles. For $\Phi = 1/2\pi$ (isotropic "scatter"), it can easily be seen that only one "constant" function of the type $H_0 = G(P, t)$ can be realized.

Next, the function Φ is assumed to be such that Eq. (7) has a unique (within a constant factor) nontrivial solution, and this is the main requirement on the function Φ in this section.

Thus, $H_0 = G(P, t)$. In accordance with (5) and (6), the next approximation with respect to ε gives the expression

$$\int_{-\pi}^{\pi} \Phi H_1 \, d\beta - H_1 = [\cos (\varphi) \, \partial G/\partial x + \sin (\varphi) \, \partial G/\partial y]/\nu . \tag{8}$$

The solution of problem (8) is sought in the form

$$H_1 = H_1^0 (P, t) + H_1^c (P, t) \cos (\varphi) + H_1^s (P, t) \sin (\varphi) . \tag{9}$$

We substitute (9) into (8), multiply (8) by cos φ, integrate the resultant equation within the limits $(-\pi, \pi)$, and then multiply (8) by sin φ and integrate it between the same limits. These operations results in the following system of linear equations for the functions H_1^c and H_1^s:

$$H_1^c \Phi_{cc} + H_1^s \Phi_{cs} = H_1^c + \nu^{-1} \partial G/\partial x , \quad H_1^c \Phi_{sc} + H_1^s \Phi_{ss} = H_1^s + \nu^{-1} \partial G/\partial y , \tag{10}$$

where

$$\Phi_{cc} = \pi^{-1} \int_{-\pi}^{\pi} \cos(\varphi)\, d\varphi \int_{-\pi}^{\pi} \Phi \cos(\beta)\, d\beta ; \quad \Phi_{cs} = \pi^{-1} \int_{-\pi}^{\pi} \cos(\varphi)\, d\varphi \int_{-\pi}^{\pi} \Phi \sin(\beta)\, d\beta ;$$
$$\Phi_{sc} = \pi^{-1} \int_{-\pi}^{\pi} \sin(\varphi)\, d\varphi \int_{-\pi}^{\pi} \Phi \cos(\beta)\, d\beta ; \quad \Phi_{ss} = \pi^{-1} \int_{-\pi}^{\pi} \sin(\varphi)\, d\varphi \int_{-\pi}^{\pi} \Phi \sin(\beta)\, d\beta . \tag{11}$$

Thus, the coefficients Φ_{cc}, Φ_{ss}, Φ_{cs}, and Φ_{sc} are the first terms of the double Fourier series of the function Φ, which determines the probability of "scatter" of the particles in a certain direction. In the general case, the function Φ is not assumed to be symmetric relative to the angular variables, and therefore, it should be considered that in a typical case $\Phi_{cs} \neq \Phi_{sc}$. Also introducing the notation

$$D_{xx} = (1 - \Phi_{ss})/(2\nu\Delta) , \quad D_{xy} = \Phi_{cs}/(2\nu\Delta) , \quad D_{yx} = \Phi_{sc}/(2\nu\Delta) ,$$
$$D_{yy} = (1 - \Phi_{cc})/(2\nu\Delta) , \quad \Delta = (1 - \Phi_{cc})(1 - \Phi_{ss}) - \Phi_{sc}\Phi_{cs} \tag{12}$$

for the diffusion coefficients, we write solution (10) in the form

$$H_1^c = -2D_{xx}\frac{\partial G}{\partial x} - 2D_{xy}\frac{\partial G}{\partial y} , \quad H_1^s = -2D_{yx}\frac{\partial G}{\partial x} - 2D_{yy}\frac{\partial G}{\partial y} . \tag{13}$$

Now, we turn to the formula of the approximation ε^2 following from (5) and (6):

$$\frac{\partial G}{\partial t} + \cos(\varphi)\frac{\partial H_1}{\partial x} + \sin(\varphi)\frac{\partial H_1}{\partial y} + \nu H_2 = \nu \int_{-\pi}^{\pi} \Phi H_2\, d\beta . \tag{14}$$

Expression (14) is integrated over φ between $(-\pi)$ and (π), taking into consideration relations (1), (9), and (13). After some manipulations, we obtain the sought transfer equation of diffusion type:

$$\frac{\partial G}{\partial t} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial G}{\partial x} + D_{xy}\frac{\partial G}{\partial y}\right) + \frac{\partial}{\partial y}\left(D_{yx}\frac{\partial G}{\partial x} + D_{yy}\frac{\partial G}{\partial y}\right) . \tag{15}$$

Thus, the quantities D_{xx}, D_{xy}, D_{yx}, and D_{yy} introduced in relations (12) are none other than but components of the two-dimensional matrix of diffusion coefficients. It should be noted that in the general case diffusion propagation of particles is anisotropic, i.e., it is not necessary that $D_{xy} = D_{yx} = 0$ and $D_{xx} = D_{yy}$.

After we obtained the diffusion equations, it is of some interest to elucidate how the coefficients of the derived relations are consistent with the basic principles of existing general theories. In the present case linear irreversible thermodynamics with its requirements on the matrix of kinetic coefficients can be such a theory. In particular, this is the condition of positive definiteness of the matrix of diffusion coefficients, which is connected with entropy production [22, 23]. However, it should be verified that

$$D_{xx} > 0 , \quad D_{yy} > 0 , \quad D_{xx}D_{yy} > (D_{xy} + D_{yx})^2/4 , \tag{16}$$

as follows from Sylvester's criterion [24] for the positive definiteness of the matrix of a bilinear form. It can be checked that constraints (16) are equivalent to the conditions $\Phi_{cc} < 1$, $\Phi_{ss} < 1$, $\Delta > 0$, which are satisfied in the typical situation.

As an example, we consider the simplest (isotropic and homogeneous in the space) case with constant functions Φ and μ: $\Phi = 1/2\pi$ and $\mu = 1/\lambda$. In dimensional form Eq. (15) is written as follows:

$$\frac{\partial G}{\partial T} = D\left(\frac{\partial^2 G}{\partial X^2} + \frac{\partial^2 G}{\partial Y^2}\right), \quad D = \frac{C\lambda}{2}. \tag{17}$$

Thus, in the present case, the diffusion properties of the medium are characterized not by a matrix with four components, but by one coefficient D, i.e., the matrix becomes a multiple of the unit matrix. It should be noted that a constant diffusion coefficient can also be realized for certain variable functions Φ and μ. For example, if the equalities $\Phi_{cs}(P, T) = \Phi_{ss}(P, T) = 0$, $1 - \Phi_{cc}(P, T) = 1 - \Phi_{ss}(P, T) = C/[2D\mu(P, T)]$, where D = const is the diffusion coefficient, hold, then this statement follows from formulas (12) and (4). It should be noted that formula (17) for the diffusion coefficient coincides with the corresponding formula from elementary transfer theory [25].

3. Equations of Hyperbolic Type as a Particular Case of the Two-Dimensional (in the Coordinates) Transfer Equation. A goal of the derivation and analysis of expressions of the type (3) formulated in [4] was to obtain (on their basis, as particular cases under certain conditions) relations of standard diffusion form containing terms of the form $\partial^2 G/\partial T^2$, or more exactly, to construct equations of diffusion, heat conduction, etc. that describe propagation of perturbations with a finite velocity. Relations (15) and (17) obtained above give an infinite rate of mass (energy) transfer. This can be explained by the fact that in Sec. 2 we considered the process at rather long times $T >> \lambda/C$, when a particle had time to interact many times with elements of the medium. Here we obtain certain hyperbolic equations (systems) as particular cases of Eq. (3). They are asymtotically correlated with relations in Sec. 2. Such a transition of solutions of hyperbolic heat- and mass-transfer equations into solutions of parabolic equations at long times has been repeatedly reported in the literature [2].

From an analysis of expressions of the type (3), only in the one-dimensional case was a relation of the "conventional" form obtained:

$$a\partial^2 G/\partial T^2 + b\partial G/\partial T = \partial^2 G/\partial X^2 \quad (a, b \ - \ \text{const}), \tag{18}$$

which is ordinarily used in description of processes with a finite velocity of propagation of perturbations. In the two- and three-dimensional cases the frequently used form of relations of the type (18) with the term $\partial^2 G/\partial X^2$ replaced by the Laplacian of the required order did not follow from an expression of the type (3) [4] in the general case. Only with a special form of the "scatter" function Φ were analogs of differential equation (18) obtained (in a sense) in the two- and three-dimensional (in the coordinates) cases that describe propagation of the "signal" with a finite velocity C.

Previous results and formula (9) show that it is reasonable to seek a solution of Eq. (3) in the form of a Fourier series in the variable φ. If we take the first three terms of the form (9) and then use ideas of Galerkin's method, we obtain the simplest system of equations of hyperbolic type. Let

$$H = G(P, T) + A(P, T)\sin(\varphi) + B(P, T)\cos(\varphi). \tag{19}$$

Having substituted (19) into (3) and integrated the result over φ between $(-\pi)$ and (π), considering the residue to be orthogonal to the first, "constant" function, we find

$$\partial G/\partial T + 0.5C\,[\partial A/\partial Y + \partial B/\partial X] = 0. \tag{20}$$

Next, we additionally multiply (3) (substituting (19) into it) by sin (φ) and integrate over φ between the same limits. As a result we obtain

$$\partial A/\partial T + C\partial G/\partial Y + \mu C\Phi_{sc}B = \mu C\,(\Phi_{ss} - 1)\,A. \tag{21}$$

After similar manipulations with cos (φ), we find

$$\partial B/\partial T + C\partial G/\partial X + \mu C\Phi_{cs}A = \mu C\,(\Phi_{cc} - 1)\,B, \tag{22}$$

where the parameters Φ_{cc}, Φ_{sc}, Φ_{cs}, and Φ_{cc} are defined by formulas (11). It can easily be seen that if terms containing the differential operator $\partial/\partial T$ are omitted in expressions (21) and (22), then, solving system (21) and (22) for A and B and substituting the result into (20), we arrive at Eq. (15) for the function G. System (20)-(22) is of hyperbolic type, and we can verify by the standard method [26] that the characteristics, i.e., the surfaces $\chi(X, Y, T) = 0$, satisfy the characteristic equation

$$\frac{\partial \chi}{\partial T}\left\{\left(\frac{\partial \chi}{\partial T}\right)^2 - \frac{C^2}{2}\left[\left(\frac{\partial \chi}{\partial X}\right)^2 + \left(\frac{\partial \chi}{\partial Y}\right)^2\right]\right\} = 0. \tag{23}$$

It can be seen from (23) that the system of differential equations (20)-(22) has a maximum characteristic velocity $2^{-1/2}C$, which does not coincide with the expected value C (it is less than this value). This can probably be attributed to the fact that Galerkin's method is approximate, and it is quite probable (below, this statement will be proved for five functions in Galerkin's series) that when a large number of terms are retained in Fourier series (19), the velocity of propagation of perturbations increases and it approaches C as the number of terms increases, remaining less than C.

In the simplest situation $\Phi = 1/2\pi$, $\mu = 1/\lambda = \text{const}$, instead of (17), from system (20)-(22) one can obtain the following equation:

$$\tau_* \frac{\partial^2 G}{\partial T^2} + \frac{\partial G}{\partial T} = D\left(\frac{\partial^2 G}{\partial X^2} + \frac{\partial^2 G}{\partial Y^2}\right), \quad \tau_* = \frac{\lambda}{C}, \quad D = \frac{C\lambda}{2}. \tag{24}$$

which already has a "classical" form [2]. Apart from this fact, a strength of expression (24) is the fact that in the extreme situation $\tau_* \to 0$, it becomes asymptotically justified relation (17) (etc. in a more general case). A weakness of this expression is that the velocity of propagation of perturbations is smaller than C. Thus, as approximations of initial expression (3), Eq. (24) and, in a more general case, system of equations (20)-(22) have a larger range of validity with respect to time than (17).

The following approximation of Galerkin's method for five "trial functions" in an expansion of the type (19) supplemented with terms of the form $A_s(P, T) \sin(2\varphi) + B_c(P, T) \cos(2\varphi)$ is of some interest. Here, we have only an analog of an equation of the type (24) for the function G for a steady homogeneous isotropic space ($\Phi = 1/2\pi$, $\mu = 1/\lambda = \text{const}$). After some manipulations, we have

$$D\left(\frac{3}{2}\tau_* \frac{\partial}{\partial T} + 1\right)\Delta_{XY} G = \left(\tau_* \frac{\partial}{\partial T} + 1\right)^2 \frac{\partial G}{\partial T}, \tag{25}$$

where Δ_{XY} is the two-dimensional Laplace operator with respect to the index variables X and Y. It can be shown that Eq. (25) contains a maximum characteristic velocity equal to $C \cdot 3^{1/2}/2$, which is closer to C than the corresponding velocity in Eq. (24). This is consistent with the aforementioned suggestion. It should be noted that derivatives of the third order appear in Eq. (25). It is likely that in derivatives of higher order will be present the equations for subsequent approximations.

NOTATION

A, B, A_s, B_c, components (functions) of the solution by Galerkin's method; a, b, constant coefficients in Eq. (18); C, velocity of propagation of particles; D, D_{xx}, D_{xy}, D_{yx}, D_{yy}, diffusion coefficients; $G(P, t)$, abbreviated notation for H_0; H, conditional probability of transition of a particle from one state to another; H^*, value of the function H with special initial data; H_j, components of the expansion into series (6) in powers of ε; H_1^0, H_1^c, H_1^s, defined by (9); J, conditional probability (defined in the text); L, characteristic spatial scale; $P(X, Y)$, $Q(\xi, \eta)$, coordinates of the particle; T, t, dimensional and dimensionless time; $\mathbf{u}$, $\mathbf{v}$, vectors (unit) of the direction of the particle velocity; X, Y, Z, x, y, Cartesian spatial coordinates; Δ, defined by (12); $\delta(z)$, delta-function; $\varepsilon = \lambda/L$, small parameter; Φ, μ, functions determining the properties of the medium; Φ_{cc}, Φ_{ss}, Φ_{cs}, Φ_{sc}, first coefficients of the expanation of the function Φ into a double Fourier series; φ, ψ, angular coordinates; λ, scale of the mean free path of a particle; ν, dimensionless value of μ according to (4); τ, time coordinate; τ_*, "relaxation time" (24); χ, characteristics of system (20)-(22).

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