

ENERGY METHOD FOR PROBLEMS OF DIFFUSION IN A MOVING MEDIUM

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UDC 536.75

Formulation of the Problem. The problems of diffusion of a substance in a moving medium arise in very different fields of natural science, for example, in mathematical simulation of the dynamics of ionospheric inhomogeneities or of the process of propagation of pollutants in the atmosphere.

In accordance with [1], the diffusion equation for small concentrations of an admixture has the form

$$\operatorname{div}(\rho \mathbf{u} C) - \operatorname{div}(\rho D \operatorname{grad} C) = Q, \quad (1)$$

where C is the mass fraction of the admixture, ρ is the density of the admixture, $\mathbf{u} = (u, v)$ is the velocity vector, D is the diffusion coefficient, and Q is the density of the admixture source. The Cartesian coordinates x, y are used.

The diffusion coefficient considered is a scalar, but all results are also valid for the symmetric, positive-definite tensor D .

Equation (1) holds in a two-dimensional domain Ω with boundary Γ . Only the function $C(x, y)$ is unknown.

If a substance that absorbs completely an admixture is outside the boundary, then the admixture concentration at the boundary is zero. Let us write this condition for a more general inhomogeneous variant:

$$C \Big|_{\Gamma} = C_0(l), \quad (2)$$

where l is a coordinate along the boundary curve Γ .

In the steady-state case, the density and the velocity satisfy the equation of continuity

$$\operatorname{div}(\rho \mathbf{u}) = 0. \quad (3)$$

From thermodynamic considerations, the diffusion coefficient is strictly positive, and Eq. (1) is, therefore, elliptic. The operator of the boundary-value problem (1) and (2) is nonsymmetric. Therefore, the principle of minimum quadratic energy functional, which allows one to use the most effective methods of approximate and numerical solution of problems with symmetric operators [2], is not valid for this operator. The thermodynamic principles of nonequilibrium processes, like the principle of production of minimum entropy, etc. cannot be formulated for such problems [3].

The purpose of the present paper is to formulate the original problem as a problem with a symmetric positively defined operator and to substantiate the corresponding energy principles.

Similar results for electric-conduction problems in which the nonsymmetry is due to the Hall effect have been obtained by the author in [4–6]. The energy principles made it possible to create economical numerical methods for solving the problems numerically and to solve some problems of ionospheric physics which cannot be solved by traditional methods [7].

Description of Transport by Gyrotropic Diffusion. By virtue of (3), for flow, a stream function $\beta(x, y)$

$$\rho \mathbf{u} = - \operatorname{rot} \beta, \quad (4)$$

Computing Center, Siberian Division, Russian Academy of Sciences, Krasnoyarsk 660036. Translated from *Prikladnaya Mekhanika i Tekhnicheskaya Fizika*, Vol. 38, No. 2, pp. 32–39, March–April, 1997. Original article submitted September 11, 1995; revision submitted November 23, 1995.

can be constructed where β is the z component of the vector $(0, 0, \beta)0$ and rot has the x and y components. Since the function β can be easily constructed from a given distribution of ρu , we regard it as a spherical function.

Equation (1) then takes the form

$$-\text{div} \left(\begin{pmatrix} \rho D & -\beta \\ \beta & \rho D \end{pmatrix} \begin{pmatrix} \partial C / \partial x \\ \partial C / \partial y \end{pmatrix} \right) = Q. \quad (5)$$

This equation has the same form as the law of conservation of charge if C is the electric potential, ρD and β are the Pedersen and Hall conductivities, respectively, and Q is the density of the source of current.

We denote the tensor of coefficients by σ . It is symmetric only for $\beta = 0$, when the material is at rest. The symmetric part of σ is positively defined.

The vector

$$\mathbf{j} = -\sigma \text{grad } C \quad (6)$$

is similar to the electric-current density for Eq. (5) but does not coincide with the true admixture flow, whose divergence is given by Eq. (1). The admixture flow is equal to $\mathbf{j} - \text{rot}(\beta C)$. The difference has zero divergence and precisely owing to this circumstance, we succeeded in writing the law of conservation of admixture mass (1) as a law of conservation for a certain auxiliary transfer process which occurs according to (6).

As its component-by-component form in (5) shows, the tensor σ is invariant under rotation about the z axis, because it itself specifies the rotation about this axis and the isotropic tension. Therefore, (6) is a diffusion law in a gyrotropic medium.

By analogy with the electrical-conduction problems, we denote

$$\mathbf{E} = -\text{grad } C. \quad (7)$$

Since rot of grad is identically equal to zero, the vector \mathbf{E} satisfies the expression $\text{rot}_z \mathbf{E} = 0$.

Construction of \mathbf{E} is equivalent to construction of $C(x, y)$ if we specify additionally the average value of C over Ω or Γ . Therefore, the original problem (1) and (2) can be replaced by the following problem:

$$\text{div } \mathbf{j} = Q, \quad \text{rot}_z \mathbf{E} = G, \quad \mathbf{j} = \sigma \mathbf{E}, \quad E_l \Big|_{\Gamma} = g(l). \quad (8)$$

Here the second equation is inhomogeneous for generality, although usually $G \equiv 0$. The boundary condition is obtained by differentiating (2) along the boundary. As noted above, the average value of the function $C_0(l)$, which vanishes in this case, will be used to construct $C(x, y)$ after solving problem (8).

Having integrated the second equation of (8) over the entire domain and the boundary condition over the whole boundary, we obtain the following condition which is necessary for the solution of problem (8):

$$\iint G dx dy = \oint g dl. \quad (9)$$

For $G = 0$ and with the constructed function g , this condition is satisfied automatically. In the general case, we assume that the specified functions G and g are subject to this condition and that the integrals of the squares of the given functions Q , G , and g are finite. The latter condition can be replaced by a weaker condition of divergence [2], which admits the presence of sources concentrated on straight lines.

Problems of gyrotropic diffusion of the form (8) or problems with other boundary conditions can arise regardless of problem (1) and (2). The direction of rotation about the z axis, which was selected for σ , can be related to the magnetic intensity vector oriented along z if the diffusing particles are charged or with the z -oriented angular-velocity vector of rotation of the medium.

The Energy Principle. Like the operator of the original problem (1) and (2), the operator of the boundary-value problem (8) is nonsymmetric. However, a symmetric formulation of such problems is proposed in [4]. Here we just formulate the results, since the method of symmetrization with appropriate proofs is described in detail in [6].

Let us introduce two new unknown functions F and P in terms of which the old unknowns \mathbf{j} and \mathbf{E}

are expressed by the formula

$$\mathbf{j} = \sigma \mathbf{E} = -\frac{1}{\sigma_0} \sigma S \sigma^t \text{grad } F + \sigma S \text{rot } P, \quad (10)$$

where P is the z component of the vector $(0, 0, P)$, S is an arbitrary symmetric and uniformly and positively defined tensor with bounded coefficients, σ_0 is a nondimensionalizing constant, and the superscript t denotes transposition.

The best estimates were obtained for

$$S^{-1} = (\sigma + \sigma^t)/(2\sigma_0), \quad \sigma_0 = \sqrt{\xi_1 \xi_2}. \quad (11)$$

Here the constants ξ_1 and ξ_2 are such that the conditions $0 < \xi_1 \leq \rho D$ and $\rho D + \beta^2/(\rho D) \leq \xi_2$ are satisfied uniformly in the domain Ω .

We consider the set of pairs of functions F and P subject to the following conditions:

$$F|_{\Gamma} = 0, \quad \iint_{\Omega} P dx dy = 0. \quad (12)$$

Let us introduce the following energy scalar product:

$$\left[\begin{pmatrix} F \\ P \end{pmatrix}, \begin{pmatrix} F' \\ P' \end{pmatrix} \right] = \iint \begin{pmatrix} \text{grad } F \\ \text{rot } P \end{pmatrix}^t \begin{pmatrix} (1/\sigma_0^2) \sigma S \sigma^t & -(1/\sigma_0) \sigma S \\ -(1/\sigma_0) S \sigma^t & S \end{pmatrix} \begin{pmatrix} \text{grad } F' \\ \text{rot } P' \end{pmatrix} dx dy. \quad (13)$$

The set of pairs of functions which are subject to conditions (12) and have a bounded energy norm is called the energy space of the problem.

We introduce an energy functional in the form

$$W(F, P) = \frac{1}{2} \left[\begin{pmatrix} F \\ P \end{pmatrix}, \begin{pmatrix} F \\ P \end{pmatrix} \right] - \iint (FQ/\sigma_0 + PG) dx dy + \oint P g(l) dl. \quad (14)$$

It has been proved that the energy functional has a single minimum on the functions in the energy space. The pair of functions that is responsible for a minimum value of the energy functional is a generalized solution of the following problem:

$$\text{div} \left(-\frac{1}{\sigma_0^2} \sigma S \sigma^t \text{grad } F + \frac{1}{\sigma_0} \sigma S \text{rot } P \right) = Q/\sigma_0, \quad \text{rot}_z \left(-\frac{1}{\sigma_0} S \sigma^t \text{grad } F + S \text{rot } P \right) = G; \quad (15)$$

$$\left(-\frac{1}{\sigma_0} S \sigma^t \text{grad } F + S \text{rot } P \right) \Big|_{\Gamma} = g(l). \quad (16)$$

These equations are the minimum conditions for $W(F, P)$. The boundary condition (16) is called a natural condition, because it is satisfied as a result of minimization, in contrast to the basic boundary conditions (12), which specify a set of admissible functions F and P .

Thus, the existence of a generalized solution of problem (8), which is a classical solution in the case of smoothness, was proved. The uniqueness of the classical solution of (8) was also proved in [6].

Formula (7) makes it possible to construct, with the use of the solution of problem (8), the function C up to an arbitrary additive constant. The arbitrariness arises because of differentiation of the boundary condition (2) in going to (8). For the constructed function C to be a solution of problem (1) and (2), this constant should be determined from the equality condition of the average values of the right- and left-hand sides of (2).

Symmetrization of the problem can be regarded simply as multiplication of the original operator by the conjugate operator from the right, as it is actually done to introduce potentials for unknown (usually vector) functions.

Impermeable Boundary. Two basic boundary conditions are possible for system (8): we specify the tangential component of \mathbf{E} , as in (8), or the normal component of \mathbf{j} :

$$j_n \Big|_{\Gamma} = q(l). \quad (17)$$

For gyrotropic diffusion, these conditions correspond to two basic physically realizable types of boundaries corresponding to a completely absorbing or impermeable substance.

For the original equation of diffusion in a moving medium (1), the first condition has already been shown to have the same meaning and to correspond to condition (2). Condition (17) can be written in the original notation as follows:

$$\left(-\rho D \frac{\partial C}{\partial n} + \beta \frac{\partial C}{\partial t}\right)\Big|_{\Gamma} = q(l). \quad (18)$$

If the boundary is impermeable not only for the admixture, but also for the basic substance, it is a streamline. Hence, by virtue of (4), the stream function at this boundary is constant and can be set equal to zero.

Condition (18) then takes the form

$$-\rho D \frac{\partial C}{\partial n}\Big|_{\Gamma} = q(l).$$

Thus, the impermeable boundary in the problem of diffusion of an admixture in a moving medium is described by the boundary condition (17) in the problem of gyrotropic diffusion.

For the functions F and P , in the problem (15) and (16) the natural boundary condition (16) is then replaced by

$$\left(-\frac{1}{\sigma_0^2} \sigma S \sigma^t \text{grad } F + \frac{1}{\sigma_0} \sigma S \text{rot } P\right)\Big|_{\Gamma} = q(l),$$

and the basic boundary conditions (12) are replaced by

$$P\Big|_{\Gamma} = 0, \quad \iint_{\Omega} F dx dy = 0.$$

Instead of (9), the condition

$$\iint Q dx dy = \oint q dl$$

becomes necessary for the solution of the problem.

Mixed Boundary-Value Problem. If the boundary of the domain consists of alternating sections of impermeable and admixture-absorbing substances, all impermeable sections lying along a single streamline, then the original problem can be reduced to the mixed boundary-value problem for the functions F and P .

We formulate the problem only for the case where there are four such sections, and the inhomogeneity of the problem is determined by a single number ε . This number specifies the difference between the concentrations of two sections of the boundary. The general mixed boundary-value problem has been investigated in [6].

Of four sections $(\Gamma_1, \gamma_1, \Gamma_2, \gamma_2)$, which form in this order, a closed boundary Γ , let sections Γ_1 and Γ_2 be impermeable, and sections γ_1 and γ_2 be absorbing.

Even with the zero functions $Q, G, q_{1,2}$, and $g_{1,2}$, the solution is not identically zero because of the inhomogeneity in the following condition:

$$C\Big|_{\gamma_2} = 0, \quad C\Big|_{\gamma_1} = \varepsilon. \quad (19)$$

As shown in [6], in this case, in going to the functions F and P it is reasonable to minimize the energy functional for

$$F\Big|_{\gamma_1} = \varepsilon, \quad F\Big|_{\gamma_2} = 0, \quad P\Big|_{\Gamma_1} = 0, \quad P\Big|_{\Gamma_2} = 0. \quad (20)$$

The energy functional for this problem consists only of the energy scalar product.

If we minimize this energy functional on another set of functions F_1 and P_1 that are specified by the basic boundary conditions

$$F_1\Big|_{\gamma_1} = 0, \quad F_1\Big|_{\gamma_2} = 0, \quad P_1\Big|_{\Gamma_1} = -\nu/\sigma_0, \quad P_1\Big|_{\Gamma_2} = 0, \quad (21)$$

then we solve a problem in which the total flux through the boundary of γ_2

$$\int_{\gamma_2} j_n dl = \nu \quad (22)$$

is specified rather than the difference between the concentrations at the sections of the boundary, as under conditions (20).

By virtue of the homogeneity of the first equation of (8) and the impermeability of the sections $\Gamma_{1,2}$, this flux enters the domain through the section γ_1 .

The functions \mathbf{E} and \mathbf{j} , which are the solution of the problem with condition (22), will be distinguished from the solution of the problem with condition (19) only by the common factor. The factor can be found easily by determining the flux through γ_2 in the solution with given concentration (19) or the difference between the concentrations of sections γ_1 and γ_2 in the solution with the given flux (22). Therefore, it suffices to solve only one of the problems.

One can calculate the ratio

$$\alpha = \left(\int_{\gamma_2} j_n dl \right) / \left(\int_{\Gamma_2} E_l dl \right). \quad (23)$$

The parameter α does not depend on the very values of ε or ν , because \mathbf{j} and \mathbf{E} are proportional to them. It characterizes the total permeability of the domain Ω , and is similar to the total conduction of a body as a whole in electrical-conduction problems or to the capacity of a pair of bodies in electrostatics problems.

Symmetrization allows one to obtain two-sided estimates of α [6] in a similar way as two-sided estimates of capacity are given by the Dirichlet and Thomson principles [8]. For arbitrary pairs of functions F, P and F_1, P_1 , which satisfy, respectively, (20) for $\varepsilon = 1$ and (21) for $-\gamma/\sigma_0 = 1$, the inequalities

$$\left(\frac{1}{\sigma_0} \left[\left(\begin{array}{c} F_1 \\ P_1 \end{array} \right), \left(\begin{array}{c} F_1 \\ P_1 \end{array} \right) \right] \right)^{-1} \leq \alpha \leq \sigma_0 \left[\left(\begin{array}{c} F \\ P \end{array} \right), \left(\begin{array}{c} F \\ P \end{array} \right) \right] \quad (24)$$

hold.

The better the functions F, P and F_1, P_1 minimize the energy functional, the more precise the estimates.

Condition (22) is meaningful for the original problem (1) only if sections $\gamma_{1,2}$ lie along the common streamline, as does $\Gamma_{1,2}$. In this case, when the basic substance moves not intersecting the boundary of the domain, definition (23) of the total permeability α and the method of obtaining its two-sided estimates based on (24) are valid for diffusion in a moving medium.

Thermodynamics. With coincidence of the elements $(F, P) = (F', P')$, the energy scalar product (13) assumes the quadratic form and can be written in terms of problem (8). The tensor S can be specified in the form $S^{-1} = (\Theta\sigma + \sigma^t\Theta)/(2\sigma_0)$, which is more general in comparison with (11). Here Θ is an arbitrary symmetric tensor, such that the tensor S remains uniformly and positively defined. If σ is gyrotropic, it is necessary and sufficient that Θ be uniformly and positively defined. Then we have

$$\left[\left(\begin{array}{c} F \\ P \end{array} \right), \left(\begin{array}{c} F \\ P \end{array} \right) \right] = \frac{1}{\sigma_0} \iint \mathbf{E}^t \Theta \mathbf{j} dx dy. \quad (25)$$

The solutions of problem (8), which were generated for various Θ , coincide owing to the uniqueness of the solution proved, although the functions F and P can be distinguished.

In particular, Θ can be given as a product of the unit tensor by the scalar function θ . Then the integral in (25) has the following form:

$$\frac{1}{\sigma_0} \iint (\text{grad } C)^t \rho D \theta \text{grad } C dx dy. \quad (26)$$

The nonsymmetric part of σ is not included in the quadratic form. Integral (26) can be written as the entropy-production rate:

$$\frac{1}{\sigma_0} \iint (\text{grad } C)^t \frac{\rho D}{T} \frac{\partial \mu}{\partial C} \text{grad } C dx dy$$

if we specify $\theta = T^{-1}\partial\mu/\partial C$, where T is the temperature and μ is the chemical potential [1]. With $\theta = \partial\mu/\partial C$, this integral is equal to the thermal-energy production rate by diffusion. This circumstance, by the way, accounts for the inclusion of the word *energy* into the terms scalar product (13) and functional (14).

The thermodynamic function $\theta = \partial\mu/\partial C$ depends on the admixture concentration, which is a solution of the problem, and the coefficient in the integrand quadratic form must be specified before the problem is solved. The function θ can be specified, because it does not enter the original problem for admixture concentration. We shall solve the problem setting, for example, $\theta = 1$. We construct \mathbf{E} and C using the found F and P . Since $\partial\mu/\partial C$ is a known function of C, T , one can now specify $\theta = \partial\mu/\partial C$. After this, we again solve the problem by minimizing the energy functional. The functional has changed, because $\theta \neq 1$. As a consequence, we obtain the different F and P , but the same \mathbf{E} and C . Such a two-stage solution does not seem to be reasonable in practice, but enables us to make the quadratic part of the energy functional equal to the entropy-production rate with a specified temperature distribution.

As mentioned above, for the mixed boundary-value problem in the domain bounded by a single streamline, the energy functional consists only of the quadratic part. In this case, the energy principle substantiated above can be treated as a minimization of the total entropy-production rate. The minimization is conditional, i.e., it is achieved for various concentration distributions, which can be represented in the form corresponding to formula (10):

$$-\text{grad } C = -\frac{1}{\sigma_0} S \sigma^\dagger \text{grad } F + S \text{rot } P,$$

where F and P are functions subject to conditions (12).

It should be noted that the principle of minimum entropy production for diffusion in a moving medium cannot be valid in an unconditional form, because entropy production does not depend on the motion of a medium. Introduction of the potentials F and P ensured a reasonable freedom for the functions C , similarly to the way the field-to-potential transition in electrostatics made it possible to formulate the principle of minimum field energy without the constraint "among irrotational fields." In our case, the availability itself of the function C ensures the irrotational character of $\text{grad } C$. However, the condition determined by formula (10) rather than this condition turns out to be necessary to formulate the energy principle.

In the degenerate case of diffusion in a medium at rest where the tensor σ is symmetric, we can take $S = \sigma^{-1}$. Then the problems for F and P are not connected, and F and P themselves acquire the meaning of a potential and of a stream function for a diffusing substance. For problem (1) and (2), with $G = 0$ we simply obtain $F = C$ and $P = 0$.

The energy principle substantiated above can be regarded as an extension of the principle of a minimum rate of total entropy production to diffusion processes in a moving medium, because only low-order terms are included additionally in the energy functional. This principle, however, can be completely interpreted from a thermodynamic point of view as well.

The Principle of Minimum Fluctuations. Like any bounded linear functional, by virtue of the Riesz' theorem, the set of low-order terms of the energy functional (14) can be represented as a scalar product by some fixed element in the energy space F' and P' .

Therefore, the energy functional can be transformed into the form

$$W(F, P) = \frac{1}{2} \left[\left(\begin{array}{c} F - F' \\ P - P' \end{array} \right), \left(\begin{array}{c} F - F' \\ P - P' \end{array} \right) \right] - \frac{1}{2} \left[\left(\begin{array}{c} F' \\ P' \end{array} \right), \left(\begin{array}{c} F' \\ P' \end{array} \right) \right],$$

where the quadratic part, which depends only on the differences of the functions, is immediately isolated.

Since the second term is not dependent on F and P , only the first term can be minimized. This quadratic form can be written in terms of the original problem, similarly to (26):

$$\frac{1}{\sigma_0} \iint (\text{grad } (C - C'))^\dagger \rho D \theta \text{grad } (C - C') dx dy + \text{const.} \quad (27)$$

Here C' is an exact solution.

The difference $C - C'$, i.e., the difference between the arbitrary concentration distribution and the exact

solution, can be called the concentration fluctuation. The total entropy-production rate is a measure of the intensity of fluctuations. Prior to minimization, it is necessary to eliminate the ambiguity in the determination of entropy, which corresponds to an arbitrary temperature distribution. For convenience, the tensor Θ should be taken as a unit tensor to solve the problem numerically or approximately if there are no special requirements on the accuracy of solution in a certain part of the domain [6].

Thus, the principle of minimum energy functional that we have proved can be treated as a thermodynamic principle of minimum fluctuations. The minimum is unconditional in the space of potentials F and P and conditional in the space of admixture-concentration distributions.

At first glance, this principle seems to be trivial: when the functions are equal, any measure of their difference vanishes. If the function C' could be known a priori, finding an exact solution with the use of this principle would be simple: $C = C'$. However, the function C' is not known. Therefore, neither the difference $C - C'$ nor the integral in (27) can be calculated. But one can minimize $W(F, P)$, which has already been proved to have the same effect.

Conclusions. For problems of admixture diffusion in a moving medium, diffusion problems in a gyrotropic medium at rest that have the same solutions have been formulated. This has allowed us to use the previously developed technique of symmetrization.

The principle of minimum quadratic functional has been justified. Thermodynamically, this principle is interpreted as the principle of minimum fluctuations. The entropy produced by fluctuations is a measure of their intensity. Minimization is conditional in the space of admixture-concentrations distributions and unconditional in the space of the potentials introduced. A method for obtaining estimates of the integral characteristic of diffusion in the streamline-bounded domain has been proposed.

Owing to symmetrization, new boundary-value problems have been formulated, which, in contrast to the original problems, have symmetric positive-definite operators. This makes it possible to use the most effective methods of approximate and numerical solutions.

This work was supported by the Russian Foundation for Fundamental Research (Grant 95-05-14192). The investigations presented have been partly supported by the International Scientific Foundation and the Government of Russia (Joint grant No. RKN300).

REFERENCES

1. L. D. Landau and E. M. Lifshits, *Theoretical Physics*, Vol. 6: *Hydrodynamics* [in Russian], Nauka, Moscow, (1986).
2. S. G. Mikhlin, *Variational Methods in Mathematical Physics*, Macmillan, New York (1964).
3. Yu. B. Rumer and M. Sh. Ryvkin, *Thermodynamics, Statistical Physics, and Kinetics* [in Russian]. Nauka, Moscow (1977).
4. V. V. Denisenko, "Symmetric form of elliptic equations governing transport processes in gyrotropic media," Moscow (1980). Deposited at VINITI 11.05.80, No. 4696-80.
5. V. V. Denisenko, "Variational methods for elliptic boundary-value problems describing transport processes with nonsymmetric tensor coefficients," *Prikl. Mekh. Tekh. Fiz.*, No. 3, 69-75 (1989).
6. V. V. Denisenko, *Energy Methods for Elliptic Equations with Nonsymmetric Coefficients* [in Russian]. Izd. SO RAN, Novosibirsk (1995).
7. V. V. Denisenko and S. S. Zamay, "Electric field in the equatorial ionosphere," *Planet. Space Sci.*, **40**, No. 7, 941-952 (1992).
8. O. A. Zolotov and V. P. Kazantsev, "A method of variational inequalities in electrostatics and magnetostatics," *Izv. Vyssh. Uchebn. Zaved., Elektromekh.*, No. 11, 40-44 (1987).