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CALCULATION OF THE EFFECTIVE THERMAL DIFFUSION COEFFICIENTS OF A NONLINEAR MULTIELEMENT PLASMA

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Knowledge of the transport properties of an equilibrium plasma consisting of a mixture of different chemical elements with a temperature from several thousand to several tens of thousands of degrees and with a concentration of charged particles of 10^{18}-10^{21} cm^{-3} is necessary in connection with the design of gas-phase nuclear reactors, powerful MHD generators, and thermal protection of spacecraft. In the indicated range of parameters the interaction energy of the charged particles of the plasma is of the order of the thermal energy – the plasma is nonideal. Experimental data of the transport properties of a nonideal plasma are very limited; calculation of rigorous theoretical expressions for the transport coefficients of an equilibrium plasma is possible on the condition of weak interparticle interaction; therefore, modeling approaches to the determination of the kinetic coefficients of a nonideal plasma acquire an important role.

The gasdynamics problems associated with the investigation of the flows of a nonideal plasma in the devices listed are usually solved in the approximation of local chemical equilibrium, and the plasma is assumed to be quasineutral. It is advisable in this approximation to switch from the diffusion equations of the components to the diffusion equations of the chemical elements if the number of components in the plasma is greater than the number of chemical elements. The mass flows of chemical elements and the "molecular" thermal flux are determined with the help of the introduction of effective transport coefficients in terms of the temperature gradient, the fractions of chemical elements, and the electric field in the plasma (the pressure is assumed to be constant). We emphasize that the calculation of the transport coefficients is correctly determined from the solution of a specific gasdynamics problem, which appreciably simplifies its formulation; the necessary transport properties of the plasma are compactly tabulated as a function of the pressure, temperature, and fractions of the chemical elements forming the plasma. The complete system of gasdynamics

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equations describing the flow of a chemically equilibrium plasma is discussed, e.g., in [1] (also see [2]). The effective transport coefficients are introduced in [2] actually in the approximation of an "ideal" plasma.

The effective thermal diffusion coefficients D_a^t to whose model calculation this paper is devoted are important characteristics of a multielement plasma. Taking D_a^t into account in connection with the solution of gasdynamics problems permits investigating the degree of separation of chemical elements in the plasma volume in the presence of a temperature gradient [3], which is necessary for the correct calculation of the thermal flux in the plasma. The possible instability of the steady-state solution of a system of gasdynamics equations with specified boundary conditions is another effect associated with D_a^t and characteristic of media with volume heat liberation proportional to the fraction of a chemical element (to the fraction of uranium for the plasma of a gas-phase nuclear reactor). In the simplified version for a two-element mixture in which the fields in the plasma, the motion of the plasma as a whole, and the electric current are neglected, the system consists of the diffusion equations of the chemical element and the energy equation; the values of the temperature and the fractions of the chemical element are specified on the boundaries. One can show in the one-dimensional case that "instability" of the concentration distribution of the element occurs in the linear approximation when $D_a^t > 0$; in the actual nonlinear case in which the dependence of D_a^t on the fraction of a chemical element and the temperature is taken into account, the "instability" is probably a "transition" among the different steady-state solutions which the formulation of the problem permits. It is natural that the sign, magnitude, and behavior of D_a^t are important both for the investigation of the "thermal diffusion instability" and for the separation of the chemical elements in the plasma volume.

The modeling system of the classical kinetic equations can be used for the calculation of the multicomponent diffusion coefficients (MDC) and other transport coefficients in terms of which the effective transport coefficients (see below) are expressed; the collisional integrals comprise I_e^e – the elastic collision integral which characterizes the interaction of charged particles, I_a^e – the elastic collision integral which describes the collisions of neutrals with each other and neutrals with charges, and I^{ne} – the inelastic collision integral; I_e^e can be determined if the transition from the description of the plasma with the help of the Liouville equation to its description in terms of a kinetic equation is valid, i.e., when the time equal to the inverse plasma frequency is less than the time between elastic "collisions" of charged particles – in other words, when the Coulomb interaction in the plasma is small in comparison with the thermal energy of its particles. The difficulty in choosing I_e^e is associated with the long-range nature of Coulomb forces; the hypothesis of paired collisions is not, generally speaking, applicable to charged particles; therefore, it is more correct to choose I_e^e in the Fokker–Planck form, which it is possible to justify on the basis of the Liouville equation or with the help of "wave" theory; the I_e^e of Balesk–Lenard and Kikhar–Aono reduce to the I_e^e of Fokker–Planck, and the divergence at large distances disappears in a natural way but remains at small distances. On the other hand, if one chooses I_e^e in the Boltzmann form by replacing the Coulomb potential of the interaction between charged particles by the Debye potential, then the results of the solution of this kinetic equation, for example, in the case of the calculation of the electrical conductivity and the viscosity, agree with the results of the solution of the Fokker–Planck equation [4]. Guided by this fact and bearing in mind that it is convenient to determine I_e^e and I_a^e in like manner (the latter is of Boltzmann form), I_e^e is used in Boltzmann form.

It is proposed to extend I_e^e in Boltzmann form to the case of a nonideal plasma, which is the modeling assumption; the expressions for the transport coefficients do not contain nonphysical divergences. A comparison of the electrical conductivity of a nonideal cesium plasma calculated with the help of a modeling kinetic equation determined in this way with the known experimental data shows satisfactory agreement [5], i.e., the neglected Coulomb effects evidently make a small numerical contribution to the kinetic coefficients of a nonideal plasma. Consequently, the application of a system of modeling kinetic equations to the calculation of the transport coefficients of a nonideal plasma is advisable.

The collision integral I^{ne} includes various inelastic collisions accompanied by chemical changes, charge exchange, excitation transfer, excitation of the plasma particles, etc.; these processes have an appreciable effect in many cases on the distribution functions of the plasma particles [6].

The effective diffusion coefficients in the approximation of an "ideal" plasma are introduced in [2]. It is proposed to take account of the interaction among the plasma particles in the thermodynamic forces. As is well known, the mass flow of the i-th component, $\mathbf{J}_i$, is [7]

$$\mathbf{J}_i = \frac{n^2}{\rho} m_i \sum_{j=1}^{N} m_j D_{ij} \mathbf{d}_j - D_i^t \nabla T, \tag{1}$$

$$\mathbf{d}_j = \frac{n_j m_j}{p} \nabla_T \mu_j - \frac{\rho_j}{p}\left(\mathbf{F}_j - \sum_{i=1}^{N} \frac{\rho_i}{\rho} \mathbf{F}_i\right).$$

The form (1) for $\mathbf{d}_j$ follows from the thermodynamics of irreversible processes and agrees with the form adopted in kinetic theory in the approximation of an "ideal" plasma [7]. In (1) n is the total concentration of plasma particles, p is the pressure, T is the temperature, D_{ij} are the MDC, m_i, n_i, μ_i are the mass, concentration, and chemical potential of the i-th component, $\rho_i = n_i m_i$, $\rho = \sum_{i=1}^{N} \rho_i$, N is the number of components in the plasma, D_i^t is the thermal diffusion coefficient, $\mathbf{F}_i$ is the force acting per unit mass of the i-th component,

$$\mu_i = \frac{kT}{m_i} \ln n_i + \chi_i(T) + \Delta\mu_i, \tag{2}$$

where k is the Boltzmann constant, $\chi_i(T)$ is associated with the partition function of the i-th component [7], and $\Delta\mu_i$ is the contribution to μ_i due to interaction. On the assumption of local chemical equilibrium the dependence

$$n_i = n_i(p, T, c_1, \ldots, c_{N_a-1}), \tag{3}$$

occurs, where N_a is the number of chemical elements forming the plasma, $c_a = \sum_{k=1}^{N} u_{ka} m_a n_k \Big/ \sum_{k=1}^{N} \sum_{a=1}^{N_a} u_{ka} m_a n_k$ is the mass fraction of the chemical element a, and u_{ia} is the number of atoms of the element a in the i-th component. One can derive from (1)-(3) an expression for the mass flow of the chemical element $\mathbf{J}_a$ $\left(\mathbf{J}_a = \sum_{k=1}^{N} u_{ka} m_a \mathbf{J}_k / m_k\right)$ and the effective diffusion coefficients

$$\mathbf{J}_a = \sum_{a=1}^{N_a-1} D_{ab} \nabla c_b + D_a^t \nabla T - D_a^E \mathbf{E},$$

$$D_{ab} = \sum_{i,j=1}^{N} u_{ia} m_a \frac{n^2}{\rho p} m_j^2 D_{ij} n_j \left[\frac{kT}{n_j m_j} \left(\frac{\partial n_j}{\partial c_b}\right)_{p,T,c_a \neq c_b} + \sum_f \left(\frac{\partial \Delta\mu_j}{\partial n_f}\right)_T \left(\frac{\partial n_f}{\partial c_b}\right)_{p,T,c_a \neq c_b} \right], \tag{4}$$

$$D_a^t = \sum_{i,j=1}^{N} u_{ia} m_a \left\{ \frac{n^2}{\rho p} m_j^2 D_{ij} n_j \left[\frac{kT}{n_j m_j} \left(\frac{\partial n_j}{\partial T}\right)_{p,\{c_a\}} + \sum_f \left(\frac{\partial \Delta\mu_j}{\partial n_f}\right)_T \left(\frac{\partial n_f}{\partial T}\right)_{p,\{c_a\}} \right] - \frac{D_i^T}{m_i} \right\},$$

$$D_a^E = \frac{n^2}{\rho p} \sum_{i,j=1}^{N} m_a u_{ia} m_j D_{ij} n_j z_j e.$$

The subscript f in (4) denotes that the f-th component enters into $\Delta\mu_j$. The term $\sim \sum_{i=1}^{N} \rho_i \mathbf{F}_i / \rho$ in $\mathbf{d}_j$ (see (1)) was neglected in the derivation of Eqs. (4), since the plasma is assumed to be quasineutral. Eqs. (4) for D_{ab} and D_a^t differ from the expressions given in [2] for these coefficients by the absence of terms $\sim (\partial\Delta\mu_j/\partial n_f)_T$, which are produced by the interaction of the plasma particles. Only the Coulomb interaction of the plasma particles was taken into account in the calculation of the effective transport coefficients; the charge–neutral and neutral–neutral interactions are insignificant under the conditions in question, as the estimates show.

The effective thermal diffusion (Fig. 1) and diffusion (Fig. 2) coefficients have been calculated for a plasma consisting of a mixture of potassium with uranium under the conditions existing in a gas-phase nuclear reactor (p = 500 atm, 90% U), as has been the effective thermal diffusion coefficient (Fig. 3) of a plasma consisting of a mixture of helium with hydrogen with parameters corresponding to the entry of spacecraft into the atmosphere of Jupiter (p = 100 atm, 20% H_2). The calculations are made in accordance with Eqs. (4) (curves 1 in Figs. 1-3), i.e., in comparison with [2] D_i^t is taken into account along with a correction for interaction in the thermodynamic forces (curves 2 in Figs. 1-3). As an illustration, the curves for the usual value of the thermal diffusion coefficient $D_{au}^t = \sum_{i=1}^{N} u_{ia} m_a D_i^t / m_i$ are given in Figs. 1-3.

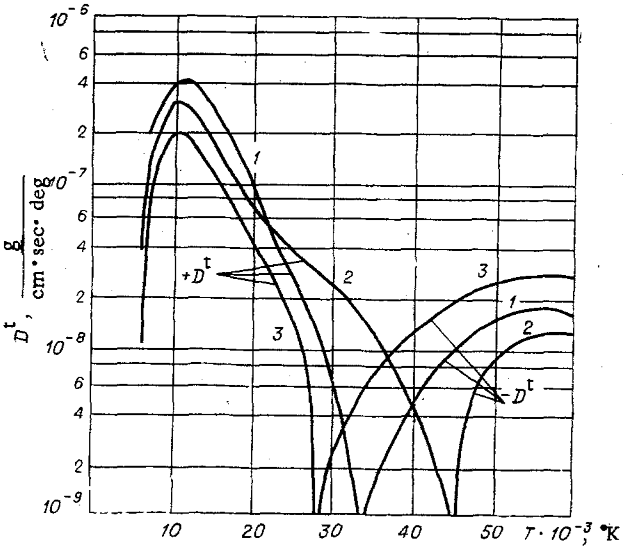

Fig. 1

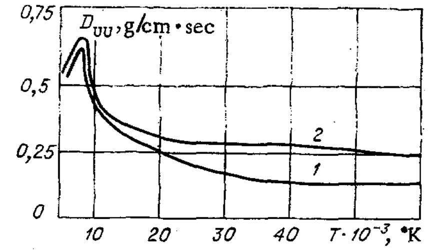

Fig. 2

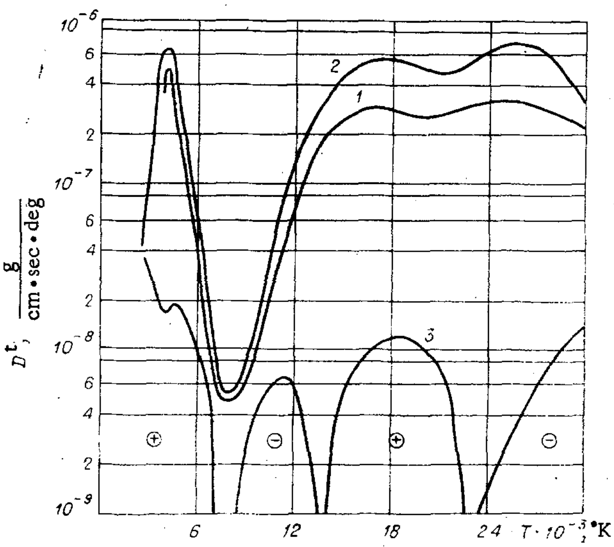

Fig. 3

All inelastic processes except charge exchanges of an atom with its own ion were neglected in the modeling system of equations with respect to the anisotropic parts of the distribution functions φ_i of the plasma particles, in terms of which the transport coefficients are defined; it was also assumed that the collision cross sections of excited particles are equal to the collision cross sections in the ground state. These simplifications, which are caused by the paucity of information about inelastic processes and by the appreciable complication of the expressions for the transport coefficients when these processes are taken into account, permit expanding φ_i in Sonin polynomials and finding D_{ij} and D_i^t normally [7]. The calculation of D_{ij} and D_i^t was carried out in the first and second approximation, respectively, in Sonin polynomials; an increase in the number of polynomials is advisable due to the simplications enumerated and a significant indeterminacy in the collision cross sections of the plasma particles of the mixtures considered in this paper.

The composition of a plasma of $He+H_2$ and K+U mixtures and the $\Delta\mu_i$ necessary for the calculation of D_{ab} and D^t_a were calculated in accordance with the procedure described in [8], and the partition function of the atoms and ions was limited to kT. Derivatives of n_i and n_f (see (4)) were calculated by a computer.

Twelve components e, K, K^-, K^+, K_2^+, K_2, K^{2+}, U, U^+, U^{2+}, U^{3+}, U^{4+} were taken into account in a plasma consisting of a mixture of uranium with potassium for temperatures ranging from 5000 to 60,000°K. The partition functions of the atoms and ions U were calculated according to the data of [9], and those of molecules, atoms, and ions of K were calculated according to the data of [10]. The interaction of the neutral components of a plasma consisting of a K+U mixture in the ground state was taken into account in accordance with [11]; the interaction of charged particles with neutral ones was assumed to be polarized; the polarizabilities of K_2 and K are given in [12], and those of U in [13]; charge exchange of a potassium atom with its own ion has been discussed in [14]. The interaction potentials and the calculation of the composition of a plasma consisting of a mixture of helium with hydrogen in the 3000-30,000°K temperature range are discussed in [2].

Taking account of interaction corrections in the thermodynamic forces during the calculation of the effective diffusion coefficients appreciably changes the size and behavior of D^t_U and D_{UU} (see Figs. 1 and 2); the Debye nonideality parameter γ lies within the range 1-3 for a plasma consisting of a mixture of K+U. The effect of $(\partial\Delta\mu_i/\partial n_f)_T$ is less appreciable for an $He+H_2$ plasma, since $\gamma\sim 0.1$-0.2 in this case. The contribution of D^t_{au} to D^t_U and D^t_{He} is also appreciable (see Figs. 1, 3); D^t_{au} is alternating for both mixtures. We emphasize that $T\cdot D^t_U\sim D_{UU}$; $D^t_{He}>0$; D^t_U is alternating in the parameter range under discussion; and D^t_U and D^t_{He} have peaks corresponding to dissociation and ionization of the plasma components. For sufficiently low temperatures condensation of uranium can occur in the K+U mixture; in this case one should refer the calculated values of D_{ab} and D^t_a to the gaseous phase.

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