NUMERICAL CALCULATION OF THE PROBLEM OF COOLING OF A SPHERICAL VOLUME OF NONEQUILIBRIUM-IONIZED RADIATING HELIUM

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The method is described and the results are presented for numerical calculations of a system of equations of nonsteady gasdynamics, radiation transfer in the continuous spectrum, and the kinetics of collisional ionization and ionization by radiation, which describe the dispersion and cooling of a spherical volume of He. A comparison is made with calculations performed on the assumption of thermodynamic equilibrium.

In the study of nonsteady gasdynamic effects in real gases it is necessary to take into account the ratio between the rates of change v_M in the macroscopic parameters E, ρ, and u and the rates v_E of processes leading to the establishment of thermodynamic equilibrium (ionization, excitation, etc.). In many problems in regions of continuous flows the inequality $v_M \ll v_E$ is satisfied. In this case each gas particle at a given time is in a state of equilibrium corresponding to the slowly varying macroscopic parameters. The quantities characterizing a real gas are functions only of E and ρ, and they can be calculated separately from the calculations of the gasdynamic motion. In regions of a sharp change in the gasdynamic quantities, such as in regions of shock waves, the criterion for the onset of equilibrium may be violated. In this case there is a nonequilibrium zone in which the state of the gas is determined by the kinetics of the physical processes taking place in it. If the extent of this zone is insignificant in comparison with the characteristic dimensions of the entire problem, where the condition of equilibrium is satisfied, then its effect on the motion of the gas as a whole can be neglected and the gasdynamics can be calculated from equilibrium theory.

With a strong decrease in v_E or an increase in v_M the equilibrium condition $v_M \ll v_E$ may be disrupted in the entire region of continuous flows. This is realized, for example, in problems of the streamline flow over bodies by a rarefied gas [1], since v_E changes sharply with a change in density, and in problems on the heating of a gas by focused radiation, when a decrease in the characteristic dimensions to fractions of millimeters leads to an increase in v_M and the fulfillment of the condition $v_M > v_E$. Because of the interaction of the kinetics and gasdynamics in these cases the joint solution of the corresponding equations is necessary. In [1] the factor simplifying the numerical calculations is the steady nature of the process. Problems on the heating of a gas by a powerful source of radiation and its subsequent dispersion, which include the studies of the present work, are nonsteady.

The process of dispersion and cooling of a spherical volume (with characteristic dimensions of ~1 mm) of high-temperature He plasma ($T \approx 10$ eV) is studied in the present work with allowance for the kinetics of ionization and energy transfer by radiation in the continuous spectrum. The stage of formation of the plasma under the effect of radiation is not considered in this case. It is assumed that its heating occurs so fast that the gas is not set into motion during the action of the radiation pulse. The system of equations describing the dispersion and cooling is close to that derived in [2], but in contrast to [2, 1] a more complex mechanism of emission and ionization processes is assumed here.

The system of gasdynamic equations has the form

$$\begin{gathered}\partial\rho/\partial t + \partial\rho u/\partial r = -2\rho u/r;\\ \partial\rho u/\partial t + \partial\rho u^2/\partial r = -\partial p/\partial r - 2\rho u^2/r;\\ \partial E/\partial t + \partial(E+p)u/\partial r = -(E+p)2u/r - q.\end{gathered} \tag{1}$$

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The following units of measurement of the quantities are adopted here and below: T, I_1, I_2, and ν, eV; $\rho_0 = 1.77 \cdot 10^{-4}$ g/cm^3; r_0, cm; $u_0 = 0.5 \cdot 10^6$ cm/sec; $t_0 = 2 \cdot 10^{-6}$ sec. The system (1) is supplemented by thermodynamic equations in which the electron excitation energy of the atoms and ions is not taken into account:

$$e = 3/2T\rho + \alpha_1 I_1 \rho + \alpha_2 (I_1 + I_2)\rho,\ p = T\rho(1 + \alpha_e),\ \alpha_e = \alpha_1 + 2\alpha_2. \tag{2}$$

The values of the nonequilibrium degrees of ionization α_1 and α_2 are determined by the following reactions: for collisional ionization $A + e \rightleftarrows A^+ + 2e$, $A^+ + e \rightleftarrows A^{++} + 2e$; for ionization by radiation $A + h\nu \rightleftarrows A^+ + e$, $A^+ + h\nu \rightleftarrows A^{++} + e$. Processes connected with the excited states of the atoms and ions and line emission are not included in the analysis. With these assumptions the equations of ionization kinetics take the form

$$\frac{\partial \alpha_0 \rho}{\partial t} + \frac{\partial \alpha_0 \rho u}{\partial r} = -\alpha_0 \alpha_e N_0 t_0 \rho^2 \sigma_0 v (I_1/T + 2) \exp(-I_1/T)(1 - L_0) - \int_{I_1}^{\infty}\int_{\Omega} \frac{C_0(\nu)}{\nu} d\Omega d\nu - \frac{2\rho\alpha_0 u}{r}; \tag{3}$$

$$\frac{\partial \alpha_2 \rho}{\partial t} + \frac{\partial \alpha_2 \rho u}{\partial r} = \alpha_1 \alpha_e N_0 t_0 \rho^2 \sigma_1 v (I_2/T + 2) \exp(-I_2/T)(1 - L_2) + \int_{I_1}^{\infty}\int_{\Omega} \frac{C_1(\nu)}{\nu} d\Omega d\nu - \frac{2\rho\alpha_2 u}{r};$$

$$\alpha_0 + \alpha_1 + \alpha_2 = 1;\ \alpha_e = \alpha_1 + 2\alpha_2;\ L_0 = \alpha_1 \alpha_e / K_1 \alpha_0;\ L_2 = \alpha_2 \alpha_e / K_2 \alpha_1;$$

$$C_{0,1}(\nu) = \alpha_{0,1} N_0 \sigma_{0\nu,1\nu} (1 - L_{0,2} \exp(-\nu/T)) \left[L_{0,2} \frac{(\exp(\nu/T) - 1) I_E(\nu)}{\exp(\nu/T) - L_{0,2}} - I(\nu, \Omega) \right];$$

$$\sigma_0 = 0.13 \cdot 10^{-17} \cdot T,\ \text{cm}^2;\ \sigma_1 = 0.41 \cdot 10^{-18} \cdot T,\ \text{cm}^2;\ v = 6.7 \cdot 10^7 \cdot T^{1/2};$$

$$K_{1,2} = (6.06 \cdot 10^{21} g_{1,2} / N_0 \rho g_{0,1}) T^{3/2} \exp(-I_{1,2}/T);$$

$$g_0 = 1;\ g_1 = 2;\ g_2 = 1;\ I_E(\nu) = C\nu^3 / [\exp(\nu/T) - 1].$$

The constant C includes the factor $2h/c^2$ and quantities which make the energy, time, and frequency dimensionless; $I(\nu, \Omega)$ is found from the radiation transfer equation, which in a nonequilibrium medium along a selected direction and in a unit frequency interval has the form

$$dI(\nu, \Omega)/ds = -\varkappa(1 - \exp(-\nu/T))(I_E(\nu) - I(\nu, \Omega)) - \varkappa_{0\nu} C_0(\nu) - \varkappa_{1\nu} C_1(\nu); \tag{4}$$

$$\varkappa_{0\nu} = \sigma_{0\nu} N_0 \alpha_0 \rho;\ \varkappa_{1\nu} = \sigma_{1\nu} N_0 \alpha_1 \rho;\ \varkappa = \varkappa_{0e} + \varkappa_{1e} + \varkappa_{2e};$$

$$\varkappa_{1e} = \sigma_{1e} N_0^2 \alpha_1 \alpha_e \rho^2;\ \varkappa_{2e} = \sigma_{2e} N_0^2 \alpha_2 \alpha_e \rho^2;\ \varkappa_{0e} = \sigma_0 N_0^2 \alpha_0 \alpha_e \rho^2.$$

The first term in (4) allows for processes of absorption and emission in free–free transitions in the fields of an atom and of singly and doubly ionized atoms. The cross sections for these processes, as for photoionization, were taken from [3]. The value used for σ_{0e} is the same as that in [4]. With the assumptions made, the expression for q in the system of gasdynamic equations (1) becomes determining:

$$q = \int_0^{\infty} \varkappa(1 - \exp(-\nu/T)) \int_{\Omega} (I_E(\nu) - I(\nu, \Omega)) d\Omega d\nu + \int_{I_1}^{\infty}\int_{\Omega} \varkappa_{0\nu} C_0(\nu) d\Omega d\nu + \int_{I_2}^{\infty}\int_{\Omega} \varkappa_{1\nu} C_1(\nu) d\Omega d\nu. \tag{5}$$

In the case of thermodynamic equilibrium the following system of algebraic equations is analyzed instead of (3):

$$\alpha_1 \alpha_e / \alpha_0 = K_1;\ \alpha_2 \alpha_e / \alpha_1 = K_2;$$

$$\alpha_0 + \alpha_1 + \alpha_2 = 1;\ \alpha_e = \alpha_1 + 2\alpha_2. \tag{6}$$

This system together with (2), with the values of E, ρ, and u assigned, determines T, α_1, and α_2. The radiation transfer equation (4) in a nonequilibrium medium is

$$dI(\nu, \Omega)/ds = -(\varkappa + \varkappa_{0\nu} + \varkappa_{1\nu})(1 - \exp(-\nu/T))(I_E(\nu) - I(\nu, \Omega)). \tag{7}$$

For the system of equations (1)-(5) we assigned the boundary conditions $\rho u = 0$ and $u = 0$ at $r = 0$; $u = 0$, $\rho = 1$, $T = 0.03$, and $\alpha_1 = \alpha_2 = 0$ at $r = \infty$ and we assumed the absence of radiation fluxes directed toward the center of the sphere. To clarify the effect of ionization nonequilibrium on the gas flow the problem, with the same initial data and boundary conditions, was calculated under two different assumptions: complete equilibrium [the system of equations (1), (2), (5)-(7)] and the absence of ionization equilibrium [the system of equations (1)-(5)], with allowance for radiation and without it.

Let us go on to a brief description of the method of the calculations. The identical form of Eqs. (1) and (3) made it possible to use the same algorithm for their solution. The basis of this algorithm is described in detail in [5]. Its simplest realization was chosen: an implicit system with an explicit antidiffusion step which does not depend on the velocity u. The solution of (1) and (3) was performed in the same space and time grids.

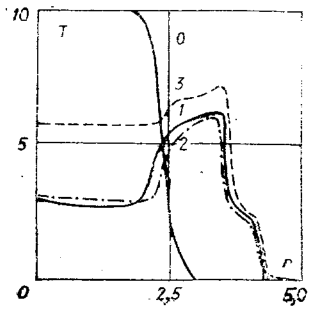

Fig. 1

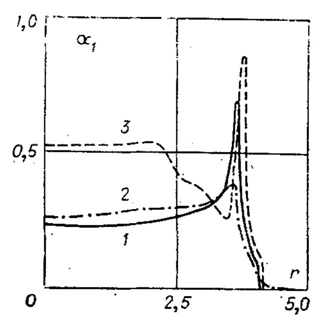

Fig. 2

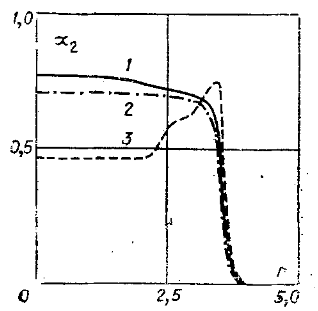

Fig. 3

The system (2), with E, ρ, u, α_1, and α_2 known at each point of space and at each moment of time from the solution of (1) and (3), determined T and p.

The emission intensity $I(\nu, \Omega)$ was found through the direct numerical solution of (4) at each point of space. Here the frequency grid was not taken as uniform but was bunched in the regions of small ν (the region of free–free transitions), of frequencies $\nu \sim I_1$ (the region of photoionization of an atom), and of frequencies $\nu \sim I_2$ (the region of photoionization of an ion). In all 30 points were taken. The grid of angles was taken as uniform and independent of the coordinate $d\theta = \pi/12$. Because of the large expenditure of machine time for the solution of the radiation transfer equation (4) it was solved with five times wider spacing than (1) or (3). The value of $I(\nu, \Omega)$ obtained in the solution of (4) for the preceding time was substituted into (1) and (3) in the intermediate time layers. In the case of complete thermodynamic equilibrium the systems (2) and (6) were solved by the iteration method.

As the initial data in the version of the calculation presented below we assigned the following values of the quantities: temperature profile (curve 0 in Fig. 1), $\rho = 1$, $u = 0$, α_1 and α_2 are the equilibrium values corresponding to these parameters, initial radius of heated region 0.375 mm. Before going on to a description of the results of the calculations, let us estimate the characteristic times for the establishment of temperature balance. The principal mechanism of temperature equalization in an ionized gas is electron collisions and the characteristic time of this reaction at the initial moment is $\sim 0.5 \cdot 10^{-10}$ sec, which is considerably less than the characteristic gasdynamic time of $\sim 10^{-8}$ sec. Therefore, the initial stage of dispersion can be considered in a one-temperature approximation. The time of establishment of ionization equilibrium at the initial moment is 10^{-9}-10^{-10} sec, i.e., the assignment of α_1 and α_2 in the equilibrium approximation is justified. The determination of the distributions of T, α_1, and α_2 at the initial time, as was indicated above, goes beyond the framework of the present report, and the algorithm constructed permits their arbitrary assignment, in particular, corresponding to exact calculations of breakdown in He.

Let us examine a direct description of the results of the calculation. The following notation are adopted in Figs. 1-5: curve 1) calculation by the theory of nonequilibrium ionization without allowance for radiation; 2) the same with allowance for radiation; 3) calculation by equilibrium theory without allowance for radiation. The coordinates $r = 1, 2, 3$, etc., correspond to the physical dimensions 0.125, 0.250, 0.375 mm, etc., and the calculating step along the coordinate equals 0.0125 mm. The temperature profiles at the time 13.6 nsec after the start of the dispersion are compared in Fig. 1. The shock wave has the coordinate 4.2 and the contact discontinuity has the coordinate 3.5. The greatest difference between curve 1 and curve 2 is in the region of $r < 2.5$. The propagation velocities of the shock wave and the contact discontinuity are about the same for all the versions of the calculations (curves 1-3), as are the distributions of ρ and u. The distribution of α_1 for the same time is presented in Fig. 2. It is seen that in the central region of flow α_{1E} in the equilibrium case is about two times larger than α_1, which is explained by a decrease in the recombination rate during collisions with a decrease in temperature and density (by this time ρ is on the order of 0.1 in the region of $r < 3$). In the region of $r > 3$ we have $\rho \sim 3$ and the ionization and recombination rates are fully adequate to maintain $\alpha_1 \approx \alpha_{1E}$. A detailed comparison of the α_1 and α_{1E} profiles is hindered, however, because these concentrations themselves depend on α_2 and α_{2E}, the relationship between which at this time is shown in Fig. 3. The tendency toward "quenching" at a lower temperature and density is displayed more clearly for this component of the gas. It is seen in Figs. 1-5 that the allowance for radiation does not strongly alter the profiles of the quantities obtained. This is explained by the fact that the temperature decreases rather rapidly and, in addition, the region is optically transparent for a large section of the spectrum $\nu < I_1$ which includes the maximum of the equilibrium radiation at temperatures below 7 eV, and therefore the radiation emanating from it is much less than the corresponding black-body radiation.

The distribution of T at the time 20 nsec is presented in Fig. 4. The shock wave has traveled to $r = 5$

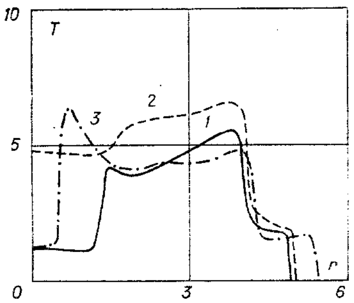

Fig. 4

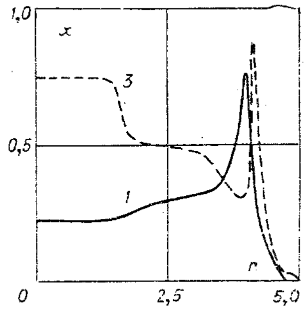

Fig. 5

and the contact discontinuity has moved to $r = 4$. About 450 calculating steps in time have been made by this time. The difference between the temperature calculated by the equilibrium theory and the nonequilibrium value is on the order of 30%. The appearance of a compression wave moving toward the center is observed on curve 1 in the region of $r < 1.4$. Curve 3 shows the distribution of T in the nonequilibrium case at a later time, 23 nsec (without radiation). The compression wave reaches almost to the center and heats the gas to 6 eV (ρ is ~0.3 at the center in this case). Such a strong wave is not observed in the equilibrium version.

The values of α_{1E} and α_1 at the time 20 nsec are compared in Fig. 5. One must conclude from the calculations presented that allowance for the nonequilibrium nature of the ionization in the problem of the cooling of a spherical volume of He with $T \sim 10$ eV, $r \sim 0.37$ mm, and a normal initial density leads, first of all, to lower temperatures averaged over the volume (by 30-40%), higher degrees of second ionization (by about two times), and, correspondingly, lower degrees of first ionization for times corresponding to dispersion to dimensions exceeding the initial dimensions by two times; secondly, it leads to the appearance of a compression wave moving toward the center, which is absent by this time in the equilibrium calculations. The ionization nonequilibrium and energy transfer by radiation do not have a significant effect on the velocity of expansion of the hot region and the propagation of the shock wave in the given calculation.

CONVENTIONAL NOTATION

u, gas velocity; ρ, density; p, pressure; E, total energy; e, internal energy; q, energy losses of matter through radiation; T, temperature of the electrons and atoms; α_0, α_1, α_2, α_e, nonequilibrium concentrations of atoms, of singly and doubly ionized atoms, and of electrons, respectively; α_{0E}, α_{1E}, α_{2E}, α_{eE}, equilibrium values of these concentrations; K_1, K_2, ionization equilibrium constants; I_1, I_2, He ionization potentials; g_0, g_1, g_2, corresponding statistical weights; $I(\nu, \Omega)$, spectral intensity of the radiation per unit frequency interval per unit solid angle; $I_E(\nu)$, its equilibrium value; ν, frequency of the radiation; $d\nu$, frequency interval; $d\Omega$, element of solid angle; N_0, Loschmidt number; M, mass of an atom; v, mean thermal velocity of the electrons; σ_0, σ_1, collisional ionization cross sections for atoms and singly charged ions; $\sigma_{1\nu}$, photoionization cross section for atoms ($\varkappa_{0\nu}$ is the corresponding spectral linear absorption coefficient); $\sigma_{0\nu}$, photoionization cross section for singly charged ions ($\varkappa_{1\nu}$); σ_{0e}, σ_{1e}, σ_{2e}, cross sections for bremsstrahlung absorption by electrons in the fields of an atom and of singly and doubly charged ions, respectively ($\varkappa_{0e}$, $\varkappa_{1e}$, $\varkappa_{2e}$).

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