$$\begin{gathered}\frac{dx_{ij}}{dt}=\frac{1}{\rho n_i}\sum_r\left(\nu'_{ir}-\nu_{ir}\right)\left[R_r(f)-R'_r(f)\right]+\\+\sum_q\left(x_{i,f-l_{iq}}\sum_{s=l_{jq}}^{W_j}x_{js}\exp\left[\frac{\theta_j}{T}l_{jq}\left(1-\frac{2s-l_{jq}}{2W_j}\right)-\frac{\theta_i}{T}l_{iq}\left(1-\frac{2f-l_{iq}}{2W_i}\right)\right]\times\right.\\\times\Omega_{f,f-l_{iq}}^{s-l_{jq},s}+x_{i,f+l_{iq}}\sum_{s=0}^{W_j-l_{jq}}x_{js}\Omega_{f+l_{iq},f}^{s,s+l_{jq}}-x_{if}\left\{\sum_{s=l_{jq}}^{W_i}x_{js}\exp\left[\frac{\theta_j}{T}l_{jq}\left(1-\frac{2s-l_{jq}}{2W_j}\right)-\right.\right.\\\left.\left.\left.-\frac{\theta_i}{T}l_{iq}\left(1-\frac{2f+l_{iq}}{2W_i}\right)\right]\Omega_{f+l_{iq},f}^{s-l_{jq},s}+\sum_{s=0}^{W_j-l_{jq}}x_{js}\Omega_{f,f-l_{iq}}^{s,s+l_{jq}}\right\}\right)+\\+\sum_q\left\{\left[x_{i,f-l_{iq}}e^{-\frac{\theta_i}{T}l_{iq}\left(1-\frac{2f-l_{iq}}{2W_i}\right)}B_q-x_{if}\right]C_q(f,f-l_{iq})-\left[x_{if}e^{-\frac{\theta_i}{T}l_{iq}\left(1-\frac{2f+l_{iq}}{2W_i}\right)}B_q-x_{i,f+l_{iq}}\right]C_q(f+l_{iq},f)\right\},\end{gathered}\tag{4.13}$$

where the quantities $R_r(f)$, $R'_r(f)$, $\Omega_{f,f'}^{s,s'}$, B_q, and $C_q(f, f')$ are determined, respectively, by the relations (2.3), (4.4), (4.9), and (4.12), (4.6). Only chemical reactions of the type (1.2) are taken into account in (4.13) in the summation over r, while only processes of the type (1.4) are taken into account in the summation over q in the first sum and only processes of the type (1.5) in the second sum.

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INFLUENCE OF NONEQUILIBRIUM OF THE CHEMICAL COMPOSITION OF A GAS ON ITS MOTION

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We consider a gas cloud in which chemical equilibrium is disturbed, which can be accomplished, for example, by a pulse of ionizing or dissociating radiation. In this case the specific thermal energy e_t can be far lower than the specific chemical energy e_c, i.e., the energy expended on breaking chemical bonds, the excitation of levels, and ionization.

In the process of relaxation of the nonequilibrium state of the gas the chemical energy is converted into thermal energy and the initially stationary gas starts to expand. The decrease in density during the dispersal causes a decrease in the rates of the chemical reactions, and the transfer of chemical into thermal energy is slowed, which in turn influences the intensity of dispersal. In such phenomena the gasdynamic processes and processes of chemical kinetics are closely connected with each other. A joint solution of the equations of gasdynamics (GD) and chemical kinetics (CK) is required for their correct description. Here the solution even of the CK equations alone causes considerable difficulties, since the corresponding system is "strict" [1]. Sufficiently effective methods of solving such systems were recently developed [2, 3]. However, for a moving gas additional difficulties

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arise in connection with the nonuniformity of the spatial density distribution.

1. We write the system of equations describing the gas motion in the absence of equilibrium:

$$\frac{\partial x_j}{\partial t} = u_j,\ \rho \frac{\partial u_j}{\partial t} = -\frac{\partial p}{\partial x_j},\ \frac{\rho}{\rho_0} = \frac{\partial x_1 \partial x_2 \partial x_3}{\partial \xi_1 \partial \xi_2 \partial \xi_3},\ \frac{\partial e}{\partial t} + p\,\frac{\partial (1/\rho)}{\partial t} = 0; \tag{1.1}$$

$$\frac{\partial n_i}{\partial t} = Q_i - \alpha_i n_i + n_i \frac{\partial}{\partial t} \ln \rho,\ \frac{\partial n_j^i}{\partial t} = -n_j^i \sum_{\mathrm{Y}} \sum_k (R_{jk}^i)_{\mathrm{Y}} + \sum_{\mathrm{Y}} \sum_k n_k^i (R_{kj}^i)_{\mathrm{Y}}; \tag{1.2}$$

$$\begin{gathered} e = e_{\mathrm{t}} + e_{\mathrm{c}},\ e_{\mathrm{t}} = \sum C_{V_i} n_i T,\ p = \sum n_i k T,\ \rho = \sum n_i \mu_i,\ n_i = \\ = \sum_j n_j^i,\ e_{\mathrm{c}} = \sum_i D_i (n_i - n_i^{\mathrm{e}}) + \sum_i \sum_k \varepsilon_k^i (n_k^i - n_k^{i\mathrm{e}}). \end{gathered} \tag{1.3}$$

Here T is the temperature; t is time; x_j are the Eulerian coordinates; ξ_i are the Lagrangian coordinates; u_j are the velocity components (j = 1, 2, 3); p is the pressure; ρ is the density; C_{V_i} is the mean heat capacity of particles of the kind i in the temperature range up to T; D_i is the dissociation potential of particles of the kind i; n_i is the concentration of particles of the kind i; n_k^i is the concentration of i particles which are in the state k with an energy ε_k^i; n_i^e and n_k^{ie} are the corresponding equilibrium concentrations; $(R_{jk}^i)_Y$ is the probability of a transition from level j to level k as a result of the process Y for an i particle; Q_i and $\alpha_i n_i$ are the terms determining the creation and disappearance of particles of the kind i; μ_i is the molecular weight of an i particle. The general system is closed by the initial and boundary conditions, which for the case of the dispersal of an initially stationary gas into a vacuum has the form

$$\begin{gathered} x_j|_{t=0} = \xi_j,\ u_j|_{t=0} = 0,\ T|_{t=0} = T_0(\xi_j), \\ n_i|_{t=0} = n_i^0(\xi_j),\ n_k^i|_{t=0} = n_k^{i0}(\xi_j),\ p(\xi_0^*) = 0, \end{gathered}$$

where boundary points are marked by the index *; n_i^o and n_k^{io} are the initial concentrations and populations of levels of particles of the kind i.

In solving the CK equations for a moving gas one must know the density $\rho(t, \xi_j)$. The task is also greatly complicated by the fact that the CK equations must be solved at a large number of points of space in accordance with the "gasdynamic" partitioning of the region of gas under consideration. Of course, a calculation of the entire problem will be too laborious in such a case, even using efficient methods of solving "strict" systems.

We propose a method of solving such problems which can be provisionally called the method of an "effective adiabatic index." The effective adiabatic index γ is defined by analogy to equilibrium thermodynamics:

$$\gamma = 1 + pv/e,\ v = 1/\rho. \tag{1.4}$$

The essence of the method consists in splitting the system (1.1)-(1.3) with respect to physical factors, which are considered separately. In the given case Eqs. (1.1) and (1.4), or the GD equations and the system (1.2), (1.3), or the CK equations are considered separately. They are connected through the functions $\gamma(t, \xi_j)$ and $\rho(t, \xi_j)$. The function $\rho(t, \xi_j)$ is used to calculate the CK equations and to obtain the function $\gamma(t, \xi_j)$ from (1.4), while $\gamma(t, \xi_j)$ is used to calculate the GD equations and determine the function $\rho(t, \xi_j)$ used in the CK system. Thus, the general system is divided into two blocks, which exchange a relatively small volume of information in the process of calculation. When the quantity γ depends little on the Lagrangian coordinates ξ_j there is no need to consider the CK at each point of space at which the density $\rho(t, \xi_j)$ is found. The CK system is calculated at selected points $\tilde{\xi}_j$. The function $\gamma(t, \tilde{\xi}_j)$ is determined at the same points. At the remaining points the value of $\gamma(t, \xi_j)$ is determined by interpolation. If the value of $\gamma(t, \tilde{\xi}_j)$ varies little at neighboring points $\tilde{\xi}_j$, then the interval between them is increased. In certain cases, such as in the propagation of a shock wave through a gas, equilibrium is disrupted at the front and it is advisable to interpolate the quantity γ not over ξ_j for a given value of t but over certain combinations $\omega_s(\xi_j, t)$ connected with the motion of the shock wave front. In other cases, such as in dispersal problems, it is sufficient to interpolate over ξ_j, and it is quite evident that the number of "reference" points $\tilde{\xi}_j$ can be small.

Sometimes it is convenient to determine the effective adiabatic index $\gamma(t, \xi_j)$ at once over a certain substantial time interval, so as to eliminate exchange between the blocks at each time step.

It is convenient to use the method of successive approximations to find such a function $\gamma(t, \xi_j)$. As the first approximation one can take the function $\gamma_1(t)$ obtained in a calculation of the CK equations with an assigned law of density variation (e.g., corresponding to the inertial stage of dispersion, $\rho \sim t^{-3}$). Then considering the system of GD equations with the function $\gamma_1(t)$ and refining the law $\rho(t, \xi_j)$, we can obtain the second approximation $\gamma_2(t, \xi_j)$, etc. The use of such procedures, accelerating the calculations, requires a preliminary analysis of the concrete problems.

2. The model problem of the dispersal into a vacuum of a gas cloud in which the oxygen is fully dissociated at the time t = 0 was solved by the method of an "effective adiabatic index." The initial composition corresponded to the actual atmosphere in the density range of $2 \cdot 10^{-2}$–$2 \cdot 10^{-4}$ kg/m³, which, according to [4], allows one to be confined to the reactions presented in Table 1. Ionization and vibrational relaxation were not taken into account. The problem was solved under the assumption of spherical symmetry with uniform initial data. In this case the system of equations (1.1)-(1.3) takes the form

$$\frac{\partial r}{\partial t} = u,\ \frac{\partial u}{\partial t} = -r^2 \frac{\partial p}{\partial m},\ \frac{\partial}{\partial t}(1/\rho) = \frac{\partial u}{\partial m},\ \frac{\partial e}{\partial t} + p\frac{\partial v}{\partial t} = 0,$$

$$e = e_{\mathrm{t}} + \epsilon_{\mathrm{c}},\ e_{\mathrm{t}} = \frac{1}{\rho}\sum_i C_{V_i} n_i T,\ e_{\mathrm{c}} = \frac{1}{\rho}\sum_i D_i\left(n_i - n_i^{\mathrm{e}}\right),$$

$$p = \sum_i n_i T,\ \frac{\partial n_i}{\partial t} = Q_i - \alpha_i n_i + n_i \frac{\partial}{\partial t}\ln\rho,$$

where m is the Lagrangian mass coordinate. The initial and boundary conditions are

$$r^*|_{t=0} = R_0,\ u|_{t=0} = 0,\ T|_{t=0} = T_0,\ n_i|_{t=0} = n_i^0,\ p^* = 0.$$

The calculations were made for a sphere of initial size R_0 = 1 m and initial temperature T_0 = 200°K at densities of $2 \cdot 10^{-2}$–$2 \cdot 10^{-4}$ kg/m³.

Let us make some estimates. Suppose that only the initial thermal energy of the gas is converted into kinetic energy, while the energy expended on dissociation proves to be unused. Then the maximum velocity of dispersal is $v_m \approx 10$ m/sec. Conversely, if all the internal energy is converted into kinetic energy then $v_m \approx 10^3$ m/sec. Thus, the degree of equilibrium in the process of dispersal can be judged from the value of v_m.

An analysis of the rates of the chemical reactions enables us to conclude that for $\rho_0 = 2 \cdot 10^{-3}$ and $2 \cdot 10^{-4}$ kg/m³ the reaction of recombination in triple collisions, $O + O + M^k \rightarrow O_2 + M$, is dominant, where M is any third particle. The characteristic recombination time has the order of magnitude

$$\tau_{\mathrm{c}} \sim \frac{\mu_{O_2}^2}{K\rho^2 N_{\mathrm{A}}^2}. \tag{2.1}$$

Here K is the recombination rate constant. We have $\tau_c \approx 10$ sec for $\rho_0 = 2 \cdot 10^{-4}$ kg/m³ and $\tau_c \approx 3 \cdot 10^{-4}$ sec for $\rho_0 = 2 \cdot 10^{-2}$ kg/m³. It must be considered that Eq. (2.1) gives an understated value of τ_c in this case due to the discarding of endothermal reactions. The characteristic time of dispersal is $\tau_d \approx R_0/\sqrt{e_t}$. In our case $\tau_d \approx 3 \cdot 10^{-3}$ sec. In comparing the characteristic CK and GD times we find that a cloud with $\rho_0 = 2 \cdot 10^{-4}$ kg/m³ disperses with freezing of the degree of dissociation. In this case the effective adiabatic index is $\gamma \rightarrow 1$. If $\rho_0 = 2 \cdot 10^{-2}$ kg/m³ then $\tau_c \lessdot \tau_d$, while for $t \approx \tau_d$ the chemical energy is converted into thermal energy and dispersal begins. In this case the effective adiabatic index γ increases monotonically with time and arrives at a "plateau." But if a regime of partial freezing occurs, arrival at a plateau does not happen The quantity γ reaches a maximum and starts to decrease. At $t \gg t_d$, $\gamma \rightarrow 1$.

It should be expected that the boundary points ($m \approx M$) disperse with complete "freezing," while the central points ($m \approx 0$) disperse with a nearly equilibrium value of γ.

A regime of "partial freezing" occurs at intermediate points. With a decrease in ρ_0 the effects connected with nonequilibrium are enhanced. This is displayed in an increase in freezing and a decrease in energy release and hence in the dispersal intensity. At the limit $t \gg \tau_d$ the sphere expands in the regime of inertial dispersal.

TABLE 1

No.	Reaction	Constant	Energy yield, eV
1	$O + O_2 + M \rightarrow O_3 + M$	$K_1 = 6{,}6\cdot 10^{-35}\exp(510/T)$	+1
2	$O + O + M \rightarrow O_2 + M$	$K_2 = 3{,}8\cdot 10^{-30}T^{-1}\exp(-170/T)$	+5,1
3	$O_2 + O_2 \rightarrow O + O + O_2$	$K_3 = (18/T^{5/2})\exp(-59300/T)$	−5,1
4	$O_2 + N_2 \rightarrow O + O + N_2$	$K_4 = (6\cdot 10^{-6}/T)\exp(-59300/T)$	
5	$O_2 + O \rightarrow O + O + O$	$K_5 = (1{,}5\cdot 10^{-4}/T)\exp(-59300/T)$	
6	$O + N_2 \rightarrow N + NO$	$K_6 = 1{,}16\cdot 10^{-10}\exp(-37900/T)$	−3,3
7	$O + NO + M \rightarrow NO_2 + M$	$K_7 = 2{,}9\cdot 10^{-33}\exp(941/T)$	+3,2
8	$O + NO \rightarrow NO_2 + h\nu$	$K_8 = 6{,}4\cdot 10^{-17}$	~
9	$O + N + M \rightarrow NO + M$	$K_9 = 1{,}8\cdot 10^{-31} 1/\sqrt{T}$	+6,5
10	$O + NO \rightarrow N + O_2$	$K_{10} = 2{,}5\cdot 10^{-15}T\exp(-19500/T)$	−1,4
11	$NO + N_2 \rightarrow N_2 + O$	$K_{11} = 1{,}5\cdot 10^{-12}\sqrt{T}$	+3,3
12	$NO + O_2 \rightarrow N + O + O_2$	$K_{12} = (6{,}6\cdot 10^{-4}T^{3/2})\exp(-75377/T)$	−6,5
13	$NO + N_2 \rightarrow N + O + N_2$	$K_{13} = K_{12}$	−6,5
14	$NO + O \rightarrow N + O + O$	$K_{14} = 20K_{12}$	−6,5
15	$NO + NO \rightarrow N + O + NO$	$K_{15} = 20K_{12}$	−6,5
16	$NO + N \rightarrow N + O + N$	$K_{16} = 20K_{12}$	−6,5
17	$N + O_2 \rightarrow NO + O$	$K_{17} = 1{,}1\cdot 10^{-14}T\exp(-3150/T)$	+1,4
18	$NO + NO + O_2 \rightarrow NO_2 + NO_2$	$K_{18} = 9\cdot 10^{-39}\exp(413/T)$	1,2
19	$NO + NO \rightarrow N_2 + O_2$	$K_{19} = (0{,}8T^{5/2})\exp(-42960/T)$	1,9
20	$NO + NO \rightarrow N_2O + O$	$K_{20} = 2{,}2\cdot 10^{-12}\exp(-32100/T)$	
21	$N_2 + O_2 \rightarrow NO + NO$	$K_{21} = (15{,}1/T^{5/2})\exp(-64570/T)$	−1,9
22	$NO_2 + O \rightarrow NO + O_2$	$K_{22} = 3{,}2\cdot 10^{-11}\exp(-300/T)$	2
23	$NO_2 + O_2 \rightarrow NO + O_3$	$K_{23} = 2{,}8\cdot 10^{-12}\exp(-23400/T)$	−2,2
24	$NO_2 + NO_2 \rightarrow NO + NO + O_2$	$K_{24} = 3{,}3\cdot 10^{-12}\exp(-13540/T)$	1,3
25	$NO_2 + O + M \rightarrow NO_3 + M$	$K_{25} = 5\cdot 10^{-31}$	
26	$O + O_3 \rightarrow O_2 + O_2$	$K_{26} = 1{,}1\cdot 10^{-11}\exp(-2150/T)$	4,1
27	$O_3 + M \rightarrow O + O_2 + M$	$K_{27} = 1{,}65\cdot 10^{-9}\exp(-11400/T)$	− 1
28	$O_3 + N \rightarrow NO + O_2$	$K_{28} = 3\cdot 10^{-11}\exp(-1200/T)$	5,5
29	$O_3 + NO \rightarrow NO_2 + O_2$	$K_{29} = 9{,}5\cdot 10^{-13}\exp(-1200/T)$	2,2
30	$O_3 + NO_2 \rightarrow NO_3 + O_2$	$K_{30} = 9{,}8\cdot 10^{-12}\exp(-3520/T)$	1,1

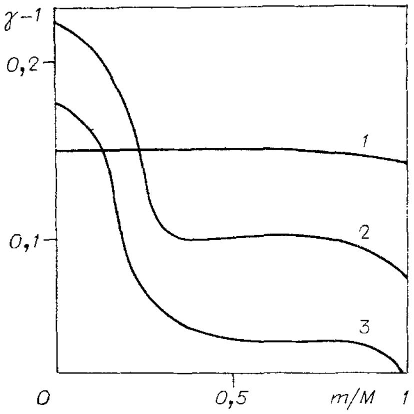

Fig. 1

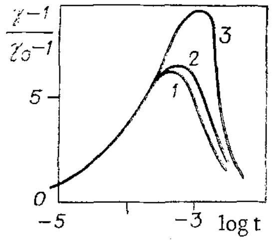

Fig. 2

The calculated function $\gamma(t, m)$ for $\rho_0 = 2\cdot 10^{-2}$ kg/m^3 is presented in Figs. 1 and 2. In Fig. 1 curves 1-3 correspond to $t = 10^{-4}$, 10^{-3}, and 10^{-2} sec. In Fig. 2 $\gamma_0 = \gamma(t = 0)$: curve 1) $m = M$; 2) $0.5M$; 3) $0.1M$ (the same in Figs. 3 and 4); $M = (1/3)\rho_0 R_0^3$ is the Lagrangian mass coordinate of the boundary of the sphere (its mass is $4\pi M$). In this example of the calculation the regime of "partial" freezing occurs for all points of the sphere. It is seen that the qualitative behavior of $\gamma(t, m)$ described above is in agreement with the calculated function.

In Fig. 3. the results of a calculation of the velocity u found in the process of solving the problem with an "exact" function $\gamma(t, m)$ (dashed lines) are compared with calculations for the equilibrium value $\gamma = 1.4$ (solid lines) for the case of $\rho_0 = 2\cdot 10^{-2}$ kg/m^3. As was estimated above, the effects connected with nonequilibrium are weakly displayed.

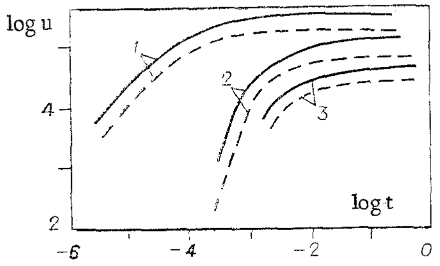

Fig. 3

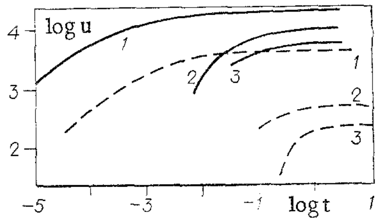

Fig. 4

In Fig. 4 we show the results of a similar calculation but for a lower initial density ($\rho_0 = 2\cdot10^{-4}$ kg/m^3). A regime close to the regime of "total freezing" occurs in this case. It is seen that the time of the start of dispersal for the real value of $\gamma(t, m)$ increases by an order of magnitude compared with the value calculated for $\gamma = 1.4$, while the velocity of dispersal for $\gamma = 1.4$ is five times higher than for the actual function $\gamma(t, m)$.

The method proved to be sufficiently effective in the examples considered. The function $\gamma(t, m)$ was determined by the method of successive approximations. Two iterations provided an accuracy of $\sim$5%, indicating rapid convergence. The system of CK equations was calculated at five points in space, which was sufficient to achieve an accuracy of $\sim$5% in the interpolations of γ. It will be interesting to extend the described method to a wider class of gasdynamic problems with strong nonequilibrium.

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ELECTROHYDRODYNAMIC PROBING OF HIGH-VELOCITY AEROSOL FLOW BY MEANS OF A CORONA DISCHARGE

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The charging of disperse aerosol particles as they move through a uniform, unipolar corona discharge whose electric field is directed along the aerosol flux was investigated in [1]. The effect of gas motion on the corona discharge characteristics, which is considerable at aerosol velocities $u \gtrsim bE$, where E is the electric field strength and b is the ion mobility, was taken into account in these investigations. On the basis of the results obtained in [1], we investigate here the macroscopic electrohydrodynamic methods of calculating the mean parameters of high-velocity aerosol fluxes in a uniform corona discharge that do not require complex microscopic measurements.

1. Consider the steady-state flow of aerosol consisting of a gas and disperse liquid particles between two flat, round grid electrodes, positioned perpendicularly with respect to the aerosol flux. Assume that in order to produce a corona discharge a system of points oriented along the aerosol flux and starting to display corona at the emitter potential $\Phi_0 > 0$ is mounted on the emitter electrode; the collector electrode is grounded (its potential

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