

MODELING OF DIFFUSION AND HEAT CONDUCTION EFFECTS ON THE VARIATION  
OF HYDRODYNAMIC PARAMETERS DURING EXCITATION OF MOLECULAR OSCILLATIONS  
BY RESONANCE RADIATION

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The necessity of investigating the laws of variation of the hydrodynamic parameters of a medium during the action of laser radiation on a resonance-absorbing medium results from the fact that these processes determine the physics of the situation in a wide class of problems of laser sounding of the atmosphere, as well as laser chemistry and technology. Studies of these laws were primarily carried out within the model of an inviscid, nonthermally conducting gas without including diffusion effects [1-6]. In the same studies, where various macrotransport processes (convection, diffusion, heat conduction) were taken into account in analyzing the hydrodynamic motion of the medium, it was assumed that internal molecular degrees of freedom are not excited during the action of radiation [7-11]. At the same time, as shown by the studies [12-15], the excitation, for example, of molecular oscillations in the gas can substantially affect processes of macrotransport.

The purpose of the present study is analysis of the effect of microtransport processes on the variation in medium parameters of the medium during resonance absorption by radiation in vibration-rotation molecular transitions.

We investigate a two-component equilibrium stationary gas mixture, consisting of diatomic molecules A(1) and B(2) with a uniform parameter distribution. Let the active radiation be absorbed at the line center of the vibration-rotation transition  $m(V', j') \rightarrow n(V'', j'')$  of molecules of kind A ( $V$  is the vibrational, and  $j$  - the rotational quantum number) at the vibrational ground state ( $V' = 0$ ) into the excited state ( $V'' = 1$ ). In this case

$$\nu_I = \nu_1 + (E_{j''} - E_{j'})/h,$$

where  $\nu_1$  is the normal oscillation frequency of molecules of sort A, while  $\nu_I$  is that of the acting radiation,  $E_{j''}$  and  $E_{j'}$  are the rotational energies of molecules of sort A in states  $n$  and  $m$ , and  $h$  is Planck's constant. Let also all molecules be found in the electronic ground state, let ionization not occur, and let there be no chemical reactions. Consider the case in which the time of induced transitions is  $\tau_I \gg \tau_{RT}$ ,  $\tau_{VV}$  ( $\tau_{RT}$  and  $\tau_{VV}$  are the characteristic times of rotation-translation and intramode vibration-vibration energy exchange). In analyzing the processes investigated in this study it can be assumed that there exists thermodynamic equilibrium between the rotational and translational degrees of freedom, while a local Boltzmann distribution is established inside each mode  $\nu_i$  ( $i = 1, 2$ ) with vibrational temperature  $T_i$  (molecular vibrations are modeled in this case by harmonic oscillators).

To describe the motion of the medium we use the system of Navier-Stokes equations for the vibrationally nonequilibrium gas, which are obtained within the first-order approximation of perturbation theory in the two-parameter distribution function from the Boltzmann kinetic equation [16, 17]:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{U}) = 0; \quad (1)$$

$$\frac{\partial N_i}{\partial t} + \nabla[N_i(\mathbf{U} + \mathbf{V}_i)] = 0; \quad (2)$$

$$\rho \frac{\partial \mathbf{U}}{\partial t} + \rho(\mathbf{U} \nabla) \mathbf{U} + \bar{\nabla} p = \sum_i N_i \mathbf{X}_i + \eta \Delta \mathbf{U} + \left( \xi + \frac{2}{3} \eta \right) \nabla(\nabla \mathbf{U}); \quad (3)$$

$$\frac{\partial}{\partial t} \left[ \rho \left( E_{RT} + \frac{U^2}{2} \right) \right] + \nabla \left[ \rho \mathbf{U} \left( E_{RT} + \frac{p}{\rho} + \frac{U^2}{2} \right) - \mathbf{U}' \sigma' + \mathbf{q}_{RT} \right] = \quad (4)$$

$$= Q_I + \sum_i \mathbf{X}_i (\mathbf{V}_i + \mathbf{U}) N_i;$$

$$\frac{\partial \rho e_i^V}{\partial t} + \nabla (\rho \mathbf{U} e_i^V) + \nabla \mathbf{q}_V^i = g_i^i + q_{VT}^i + q_{VV'}^i, \quad (5)$$

$$\mathbf{q}_{RT} = \rho T \sum_i C_{RT}^i \mathbf{V}_i - \lambda \nabla T + \frac{kT}{N} \sum_{i \neq j} \frac{D_{ij}^T N_j}{m_i D_{ij}} (\mathbf{V}_i - \mathbf{V}_j),$$

$$\mathbf{q}_V^i = \rho e_i^V \mathbf{V}_i - \lambda_i^V \nabla T_i + N k T \sum_{j=1}^2 D_{ij}^V \mathbf{d}_j,$$

$$\mathbf{V}_i = \frac{N^2}{N_i \rho} \sum_{j=1}^2 m_j D_{ij} \mathbf{d}_j - \frac{1}{m_i N_i} (D_i^T \nabla \ln T + D_i^V \nabla \ln T_i),$$

$$\mathbf{d}_j = \nabla \left( \frac{N_j}{N} \right) + \left( \frac{N_j}{N} - \frac{N_j m_j}{\rho} \right) \nabla \ln p + \frac{N_j m_j}{\rho p} \sum_i N_i \mathbf{X}_i - \frac{N_j \mathbf{X}_j}{p},$$

$$Q_I = k_\nu I \left( 1 - \frac{\nu_1}{\nu_I} \right) - \sum_i (q_{VT}^i + q_{VV'}^i), \quad q_I^i = k_\nu I \frac{\nu_i}{\nu_I} \delta_{i,1},$$

$$q_{VT}^i = -h \nu_i N_i (\varepsilon_i - \varepsilon_{ie}) \sum_j W_{i,0}^j N_j, \quad E_{RT} = C_{RT} T,$$

$$q_{VV'}^i = h \nu_i N_i L_i \frac{r_i}{g_i^{r_i}} W_{1,2} N, \quad L_1 = -L_{1,2} \gamma_2, \quad L_2 = L_{1,2} \gamma_1,$$

$$L_{1,2} = \varepsilon_1^{r_1} (\varepsilon_2 + 1)^{r_2} - \varepsilon_2^{r_2} (\varepsilon_1 + 1)^{r_1} \exp[(r_2 h \nu_2 - r_1 h \nu_1)/kT],$$

$$p = \rho R T / \mu, \quad e_i^V = \frac{h \nu_i R}{k \mu} \varepsilon_i \gamma_i, \quad C_{RT}^i = \left( \frac{3}{2} + C_R^i \right) \frac{R}{\mu} \gamma_i, \quad C_{RT} = \sum_i C_{RT}^i,$$

$$\varepsilon_i = g_i [\exp(h \nu_i / k T_i) - 1]^{-1}, \quad \varepsilon_{ie} = \varepsilon_i(T).$$

Here  $\rho$ ,  $p$ ,  $T$  are the gas density, pressure, and temperature,  $\mathbf{U}$  is the velocity of motion of the medium,  $\mu = \sum_i \mu_i \gamma_i$ ,  $\mu_i$ ,  $\gamma_i$  are the molecular masses of the  $i$ -th component and its molar fraction in the mixture,  $N_i = N \gamma_i$ ,  $N$  is the total number of particles per unit volume,  $m_i$  is the molecular mass of the  $i$ -th component of the mixture,  $R$  is the universal gas constant,  $k$  is the Boltzmann constant,  $g_i$  is the degeneracy multiplicity of mode  $\nu_i$ ,  $C_R^i = 1$  for linear and  $C_R^i = 1.5$  for nonlinear molecules,  $\lambda_i^V$  is the vibrational conductivity coefficient for the  $i$ -th component,  $\lambda$  is the heat conduction coefficient,  $D_i^T$  and  $D_{ij}$  are the thermal and multicomponent diffusion coefficients for the  $i$ -th component,  $D_{ij}^V$  is the diffusion coefficient of vibrational energy between the  $i$ -th and  $j$ -th oscillators,  $D_i^V$  is the vibrational thermal diffusion coefficient,  $\eta$  and  $\xi$  are the viscosity coefficients,  $(\mathbf{U}' \sigma')$  is the vector with components  $U_j \sigma'_{jk}$ ,  $\sigma'_{jk}$  is the viscous stress tensor,  $\mathbf{X}_i$  are external forces acting on a single particle of sort  $i$  (in the problem considered  $\mathbf{X}_i = \{m_i \mathbf{g}, \mathbf{f}_{NL}^i\}$ ,  $\mathbf{g}$  is the gravity force acceleration, and  $\mathbf{f}_{NL}^i$  is the nonlinear force acting on a particle of sort  $i$  in an electromagnetic field),  $W_{i,0}^j$  is the rate constant of vibration-translation VT-exchange for collisions of molecules of sort  $i$  with partner  $j$  ( $j = 1, 2$ ),  $W_{1,2}$  is the rate constant of intermodel vibration-vibration VV'-exchange,  $I$  is the intensity of the acting radiation,  $k_\nu$  is the radiation absorption coefficient at the vibration-rotation  $m \rightarrow n$  transition, and  $r_i$  is the number of vibrational quanta lost by the  $i$ -th partner during VV'-exchange. In writing the expressions for  $q_{RT}$  and  $q_V^i$  it has been taken into account that for a harmonic oscillator the vibration-translation conductivity coefficients are  $\lambda_i^{VT} = 0$  [18], and one also has

$$\lambda_i^V = D_{ij}^V C_{Vi}, \quad C_V^i = \left( \frac{h \nu_i}{k T_i} \right)^2 \frac{N_i k \exp(h \nu_i / k T_i)}{[\exp(h \nu_i / k T_i) - 1]^2}.$$

Since  $N_1$ ,  $N_2$ , and  $\rho$  are related by

$$\rho = m_1 N_1 + m_2 N_2, \quad (6)$$

then Eq. (1) and the two equations of the form (2) are linearly dependent. It is hence easily obtained that, along with the ordinary relations between the multicomponent and thermal diffusion coefficients  $D_{ij} = D_{ji}$  and  $D_1^T = -D_2^T$  [19], the following equality must also be satisfied

$$D_1^V \nabla \ln T_1 = -D_2^V \nabla \ln T_2. \quad (7)$$

We investigate an axially symmetric beam with a Gaussian intensity distribution in the radius  $I(r, t) = I_0(t) \exp(-r^2/R_a^2)$  with  $R_a \ll k_V^{-1}$  ( $R_a$  is the characteristic radius of the beam), while  $I_0(t) = I_0$  for  $0 < t \leq \tau_p$  and  $I_0(t) = 0$  for  $t > \tau_p$  ( $\tau_p$  is the pulse duration of the acting radiation). In this case the parameter variations in the longitudinal direction can be neglected in comparison with their variations in the transverse cross section of the beam, and can be treated as an optically thin gas film in which the action of macrotransport processes occurs only along the beam radius. Introducing the dimensionless coordinates  $r' = r/R_a$ ,  $t' = t/\tau_p$  and transforming to the new variables  $\tilde{N}_i = N_i/N_{i0}$ ,  $\tilde{U} = U\tau_p/R_a$ ,  $\tilde{\rho} = \rho/\rho_0$ ,  $\tilde{p} = p/N_0kT_0$ ,  $\tilde{T} = T/T_0$ ,  $\tilde{V}_i = V_i\tau_p/R_a$ ,  $\tilde{T}_i = T_i/T_0$ ,  $\tilde{k}_V = k_V/k_V^0$ ,  $\tilde{I} = I/I_0$  (the index zero corresponds to the moment of time  $t = 0$ ), the system (1)-(5) is reduced to dimensionless form, separating in this case the characteristic times of different transport processes (primes and tildes are henceforth omitted whenever possible)

$$\frac{\partial \rho}{\partial t} = -\nabla(\rho U); \quad (8)$$

$$\frac{\partial N_i}{\partial t} = -\nabla \left\{ N_i \left[ U - \frac{\tau_p}{\tau_{Ti}} \frac{\nabla \ln T}{N_i} - \frac{\tau_p^V \nabla \ln T_i}{\tau_{Di}^V N_i} + \frac{\tau_p}{\tau_D} \sum_k d_k \frac{N_0^2 m_k}{\rho_0 N_{i0}} \frac{N^2}{N_i \rho} \right] \right\}; \quad (9)$$

$$\rho \frac{\partial U}{\partial t} + \rho(\mathbf{UV})U = -\frac{\nabla p}{\kappa} \left( \frac{\tau_p}{\tau_a} \right)^2 + \frac{\tau_p}{\tau_c} \left[ \Delta U + \left( \frac{\xi}{\eta} + \frac{1}{3} \right) \nabla(\mathbf{VU}) \right] + \left( \frac{\tau_p}{\tau_F} \right)^2 \sum_k N_k X_k \gamma_{k0}; \quad (10)$$

$$\begin{aligned} \rho \frac{\partial E_{RT}}{\partial t} + \rho(\mathbf{UV})E_{RT} = & -p \mathbf{VU}(\kappa - 1) + \kappa(\kappa - 1) \left[ \sum_i X_i V_i N_i \left( \frac{\tau_a}{\tau_F} \right)^2 \gamma_{i0} + \right. \\ & \left. + \frac{\tau_a^2}{\tau_p \tau_c} \mathbf{VU}' \sigma' \right] + k_V I \delta \frac{\xi}{\theta_1 + \zeta} + (\kappa - 1) \sum_i \left[ \frac{\tau_p}{\tau_{iV}^T} \theta_i N_i \gamma_{i0} (\varepsilon_i - \varepsilon_{i0}) - \right. \\ & \left. - \frac{\tau_p}{\tau_{VV}'} L_{1,2} \frac{(-1)^i \theta_i r_i N_1 N_2}{g_i^r} \right] - \nabla \left[ \frac{\rho T}{C_{RT}^0} \sum_i C_{RT}^i V_i - \frac{\tau_p}{\tau_\lambda} \nabla T + \right. \\ & \left. + \frac{T}{N} \sum_{i \neq j} (V_i - V_j) (\kappa - 1) \frac{N_j \gamma_{j0} \gamma_{j0} \tau_D}{\tau_{Ti}} \right]; \end{aligned} \quad (11)$$

$$\begin{aligned} \rho \frac{\partial e_i^V}{\partial t} + \rho(\mathbf{UV})e_i^V = & \left[ \delta_{1,i} k_V I \frac{\tau_p}{\tau_I} - \frac{\tau_p N_i}{\tau_{iV}^T} (\varepsilon_i - \varepsilon_{i0}) + (-1)^i \times \right. \\ & \left. \times \frac{L_{1,2} r_i \tau_p N_1 N_2}{\gamma_{i0} g_i^r \tau_{VV}'} \right] \frac{\theta_i}{C_{i,0}^V} - \nabla \left\{ \rho e_i^V V_i - \frac{\tau_p}{\tau_i^V} \nabla T_i + \frac{NT}{C_{i,0}^V \gamma_{i0}} \sum_k \frac{\tau_p}{\tau_{ik}^V} d_k \right\}, \end{aligned} \quad (12)$$

$$V_i = -\frac{\tau_p}{\tau_{Ti}} \frac{\nabla \ln T}{N_i} - \frac{\tau_p}{\tau_{Di}^V} \frac{\nabla \ln T_i}{N_i} + \frac{\tau_p}{\tau_D} \sum_k d_k \frac{N_0 m_k N}{\rho_0 \gamma_{i0} \gamma_i \rho},$$

$$d_k = \gamma_{k0} \nabla(\gamma_k) + \gamma_{k0} \left( \gamma_k - \frac{N_k}{\rho} \frac{m_k N_0}{\rho_0} \right) \nabla \ln \rho +$$

$$+ \left( \frac{N_k}{\rho} \frac{m_k N_0}{\rho_0} \sum_j \gamma_{j0} N_j X_j - N_k X_k \right) \frac{\kappa \tau_a^2 \gamma_{k0}}{\tau_F^2 \rho},$$

$$C_{i,0}^V = \theta_i^2 \frac{\exp(\theta_i)}{[\exp(\theta_i) - 1]^2}, \quad \theta_i = \frac{h v_i}{k T_0},$$

$$\kappa = 1 + \left( C_{RT}^0 \frac{\mu_0}{R} \right)^{-1}, \quad \zeta = \frac{E_{j'} - E_j}{k T_0}, \quad \delta = \frac{k_V^0 I \tau_p}{\rho_0 C_{RT}^0 T_0} = (\theta_1 + \zeta) \frac{\tau_p}{\tau_I} (\kappa - 1) \gamma_{10}.$$

Here  $\tau_a = R_a / \sqrt{\kappa p_0 / \rho_0}$  is the propagation time of sound oscillations across the beam,  $\tau_D = R_a^2 / D_{ij}$ ,  $\tau_{Ti} = R_a^2 m_i N_{i0} / D_i^T$ ,  $\tau_{Di}^V = R_a^2 m_i N_{i0} / D_i^V$ ,  $\tau_{ij}^V = R_a^2 / D_{ij}^V$  are, respectively, the times

of multicomponent diffusion, thermal diffusion of the  $i$ -th component, vibrational energy diffusion of the  $i$ -th oscillator, and vibrational diffusion between the  $i$ -th and  $j$ -th oscillators,  $\tau_\lambda = \rho R_a^2 C_{RT}^0 / \lambda$  is the heat conduction time,  $\tau_i^V = R_a^2 C_{V_0}^i / \lambda_i^V$  is the vibrational heat conduction time of the  $i$ -th oscillator,  $\tau_i^{VT} = \left( \sum_j W_{i,0}^j N_{j,0} \right)^{-1}$  is the VT-relaxation time for the  $i$ -th oscillator,  $\tau_{VV'} = (W_{12} \gamma_{10} \gamma_{20} N_0)^{-1}$  is the VV'-exchange time,  $\tau_I = N_{10} h \nu_I / k_v^0 I_0$ ;  $\tau_k = \frac{R_a^2 \rho_0}{\eta}$  is the convection time due to viscosity, and  $\tau_F = \sqrt{\frac{\rho_0 R_a}{X_0 N_0}}$  is the time of variation of the state of the medium under the action of exterior forces  $X_0$ . According to (6), in this case we have

$$\rho = \frac{N_1 P_m + N_2 P_N}{P_m + P_N}, \quad P_m = \frac{m_1}{m_2}, \quad P_N = \frac{\gamma_{20}}{\gamma_{10}}. \quad (13)$$

Consider the case in which the absorption coefficient can be represented in the form [20]

$$k_v = k_v^0 \frac{1 - \exp(-\zeta) \varepsilon_1}{1 - \exp(-\zeta) \varepsilon_{10}}, \quad (14)$$

$$\varepsilon_{10} = [\exp(\theta_1) - 1]^{-1} g_1, \quad \varepsilon_1 = \left[ \exp\left(\frac{\theta_1 T_0}{T_1}\right) - 1 \right]^{-1} g_1.$$

It is seen from (8)-(14) that the character of variation of hydrodynamic parameters is primarily determined by the hierarchy of times  $\tau_p$ ,  $\tau_a$ ,  $\tau_D$ ,  $\tau_{Ti}$ ,  $\tau_{Di}^V$ ,  $\tau_{ij}^V$ ,  $\tau_\lambda$ ,  $\tau_i^V$ ,  $\tau_i^{VT}$ ,  $\tau_{VV'}$ ,  $\tau_I$ ,  $\tau_k$ ,  $\tau_F$  and, secondarily, by the set of dimensionless parameters  $\theta_i$ ,  $\zeta$ ,  $P_m$ ,  $P_N$ ,  $\kappa$ . We restrict this study to the case in which  $\tau_2^{VT}$ ,  $\tau_{VV'}$ ,  $\tau_k$ ,  $\tau_F \gg \max\{\tau_a, \tau_D, \tau_i^V, \tau_{Ti}, \tau_1^{VT}, \tau_I, \tau_p\}$ . Besides, it is taken into account that the coefficient  $D_{ij}^V$  is related to  $D_{ij}$ , while  $D_i^V$  is related to  $D_i^T$ . According to [12, 13, 16] one can put  $D_{ij}^V = k_V D_{ij}$  and  $D_i^V = k_V D_i^T$ , where, depending on the molecular type,  $k_V$  can vary from 0.4 to 1. We further put  $k_V = 1$ , which is characteristic of polar molecules (CO, HCl) [13]. We note that  $k_V = 0$  corresponds formally to the case in which the processes of vibrational energy diffusion, vibrational thermal diffusion, and vibrational heat conduction can be neglected (in this case  $\tau_{Di}^V$ ,  $\tau_{ij}^V$ ,  $\tau_i^V \approx \infty$ ). The times  $\tau_D$ ,  $\tau_{Di}^V$ ,  $\tau_{Ti}$ ,  $\tau_{ij}^V$ ,  $\tau_i^V$ ,  $\tau_\lambda$  are mutually dependent since the following relations hold

$$\tau_{ij}^V = k_V^{-1} \tau_D, \quad \tau_i^V = \tau_{ij}^V, \quad \tau_\lambda = \kappa \tau_D, \quad \tau_{D1}^V = k_V^{-1} \tau_{T1}, \quad \tau_{Ti} =$$

$$= \tau_D \frac{\gamma_{10}^2 (P_m + P_N)}{k_{Ti}} \left( \frac{P_N}{P_m} \right)^{i-1},$$

and, besides, it follows from (7) that

$$\tau_{D2} = -\tau_{D1}^V \frac{P_N}{P_m} \frac{\nabla \ln T_2}{\nabla \ln T_1}.$$

Here  $k_{Ti}$  are thermal diffusion ratios ( $k_{T1} = -k_{T2}$ , their values depend on  $P_m$  and  $P_N$ , and on the parameters of the intermolecular interaction potential [21]). Thus, only the following characteristic times are independent in the problem under consideration:  $\tau_a$ ,  $\tau_D$ ,  $\tau_1^{VT}$ ,  $\tau_{VV'}$ ,  $\tau_I$ ,  $\tau_p$ . In this case we have a set of independent dimensionless parameters, determining the character of variation of the hydrodynamic motion of the medium during nonuniform excitation of molecular oscillations of a single mixture component by resonance radiation:  $P_a = \tau_p / \tau_a$ ,  $P_D = \tau_p / \tau_D$ ,  $P_V = \tau_p / \tau_1^{VT}$ ,  $P_m$ ,  $P_N$ ,  $\zeta$ ,  $\theta_1$ ,  $\kappa$ ,  $P_I = \tau_p / \tau_I$ .

Let the value of energy absorption during the time of radiation action be substantially smaller than the energies of rotational and translational molecular degrees of freedom, i.e.,  $\delta \ll 1$ . One can then linearize Eqs. (8)-(12), representing  $\rho$ ,  $N$ ,  $T$ ,  $U$ ,  $V_i$ ,  $d_i$  in the form

$$Z = 1 + \delta Z', Z = \rho, N, T, N_i, U = \delta U', V_i = \delta V'_i, d_i = \delta d'_i. \quad (15)$$

It is noted that Eq. (12) is not linearized. Substituting (15) into (8)-(12), and neglecting terms of higher order than  $\delta$ , following elimination of  $U'$  from (8), (9) one obtains a system of equations for the dimensionless perturbations  $N_1'$ ,  $\rho'$ ,  $T'$  and the dimensionless vibrational temperature  $T_1 = T_1/T_0$ , describing the variation of the state of the medium for  $t \leq \tau_p$ :

$$\frac{\partial N'_i}{\partial t} = \frac{\tau_p}{\tau_D} \Delta \left( N'_i - \rho' - \frac{m_j N_{j0} N_0 (m_i - m_j)}{m_2^2 N_{10}^2 (P_m + P_N)^2} \rho' \right) + \frac{\partial \rho'}{\partial t} + \frac{m_1 m_2 k_{Ti} N_0 \tau_p}{m_i \gamma_{i0} \rho_0 \tau_D} \left\{ \Delta T' + \left( \frac{\nabla T_1}{T_1} \nabla \right) N'_i + \frac{1}{\delta} \left[ \frac{\Delta T_1}{T_1} - \left( \frac{\nabla T_1}{T_1} \right)^2 \right] \right\}; \quad (16)$$

$$\kappa \frac{\partial^2 \rho'}{\partial t^2} = \left( \frac{\tau_p}{\tau_a} \right)^2 \Delta (\rho' + T'); \quad (17)$$

$$\frac{\partial T'}{\partial t} = \frac{\zeta [1 - \exp(-\zeta) \varepsilon_1]}{(\theta_1 + \zeta) [1 - \exp(-\zeta) \varepsilon_{10}]} I + \frac{\tau_p}{\kappa \tau_D} \Delta T' + \left\{ -(\nabla V'_1 - \nabla V'_2) k_{T1} + \right. \quad (18)$$

$$\left. + \frac{\tau_p}{\delta} \gamma_{10} \theta_1 \frac{\varepsilon_1 - \varepsilon_{10}}{\tau_1^{\nabla T}} + \frac{\partial \rho'}{\partial t} \right\} (\kappa - 1) + \frac{\tau_p}{\tau_D} \left( \frac{\nabla T_1}{T_1} \nabla \right) T' \frac{m_2 k_{T1} N_0}{\rho_0} (1 - P_m);$$

$$C'_{V1} \frac{\partial T_1}{\partial t} = \frac{\tau_p}{\tau_D} \Delta T_1 + C'_{V1} \left( \frac{\nabla T_1}{T_1} \nabla \right) T_1 \frac{\tau_p m_2 N_0 k_{T1}}{\tau_D \gamma_{10} \rho_0} + \quad (19)$$

$$+ \frac{\theta_1}{C'_{1,0}} \left\{ \frac{\tau_p}{\tau_I} \frac{[1 - \exp(-\zeta) \varepsilon_1]}{[1 - \exp(-\zeta) \varepsilon_{10}]} I - \frac{\tau_p}{\tau_1^{\nabla T}} (\varepsilon_1 - \varepsilon_{1e}) \right\} - \delta \nabla d'_2 \frac{\tau_p}{\tau_D C'_{1,0}}, T_2 = 1,$$

$$V'_i = \frac{\tau_p}{\tau_D} \left\{ \frac{d'_j m_1}{\gamma_{10} (P_N + P_m) m_i \gamma_{i0}} - \frac{m_1 m_2 N_0 k_{Ti}}{m_i \rho_0 \gamma_{i0}} \nabla T' - \frac{m_1 m_2 N_0 k_{Ti}}{\delta m_i \rho_0 \gamma_{i0}} \frac{\nabla T_1}{T_1} \right\},$$

$$d'_j = (P_N + P_m) \gamma_{10}^2 (-1)^j \nabla (\rho' - N'_1) + \gamma_{j0} \left[ 1 - \frac{m_j}{m_2 \gamma_{10}} (P_N + P_m)^{-1} \right] \nabla \rho',$$

$$C'_{Vi} = C'_V / N_{i0} k C'_{i,0}.$$

The following initial and boundary conditions hold for the problem considered:

$$t = 0: \rho' = N'_1 = N'_2 = T' = 0, T_1 = 1,$$

$$\frac{\partial \rho'}{\partial t} = (P_m + P_N)^{-1} \left( \frac{\partial N'_1}{\partial t} P_m + \frac{\partial N'_2}{\partial t} P_N \right),$$

$$r = 0: \frac{\partial \rho'}{\partial r} = \frac{\partial N'_1}{\partial r} = \frac{\partial N'_2}{\partial r} = \frac{\partial T'}{\partial r} = \frac{\partial T_1}{\partial r} = 0,$$

$$r = \infty: \rho' = N'_1 = N'_2 = T' = 0, T_1 = 1.$$

It is noted that the initial condition for  $\partial \rho' / \partial t$  follows from (13). The two equations of the form (15), as well as (17)-(19), completely determine the variation of all hydrodynamic parameters for known  $P_a$ ,  $P_D$ ,  $P_V$ ,  $P_I$ ,  $P_m$ ,  $P_N$ ,  $\zeta$ ,  $\theta_1$ ,  $\kappa$  values. The numerical integration of this system of equations was carried out by using implicit difference schemes of second order accuracy in space and first order accuracy in time [22]. It was assumed that the conditions at infinity are satisfied at some finite  $r = R_b$ , whose value depends on  $P_a$  and is determined by the condition of including the effect of perturbation reflection from a fictitious exterior boundary for the parameters at the beam center. In modeling the effect of macrotransport processes on the variation of hydrodynamic parameters we assume that  $\tau_p = \tau_1^{\nabla T}$  ( $P_V = 1$ ) and  $\kappa = 1.4$ . It has been assumed that the character of molecular interactions is determined by the Lennard-Jones potential [21] with typical parameters for diatomic molecules  $\sigma = 2.8 \cdot 10^{-8}$  cm,  $\varepsilon = 3 \cdot 10^{18}$  erg.

Consider initially the effect of processes related to excitation of molecular oscillations. Figure 1 shows for  $P_a = 10$ ,  $P_I = P_D = 1$  the variation in  $N_1'$ ,  $N_2'$ ,  $N'$ ,  $T'$ , and  $T_1$

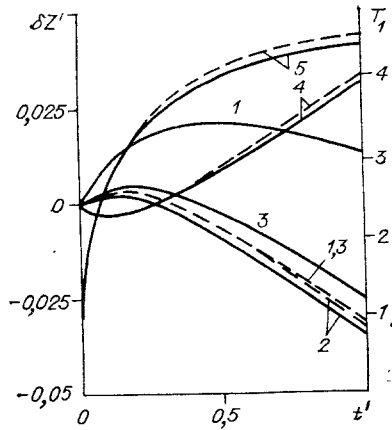


Fig. 1

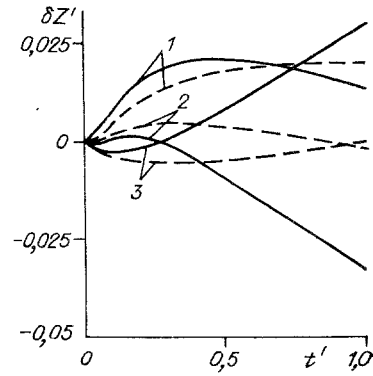


Fig. 2

(lines 1-5) with time  $t' = t/\tau_D$  on the beam axis for  $P_m = 0.5$ ,  $P_N = 4$ ,  $\zeta = -1$ , and  $\theta_1 = 7$  [the solid lines correspond to the complete model, and the dashed - to the model in which macrotransport processes related to excitation of vibrational degrees of freedom are not taken into account ( $k_V = 0$ )]. For the parameter values utilized we have the following time relations:  $\tau_I = \tau_D = \tau_{ij}^V = \tau_i^V = \tau_1^V T$ ,  $\tau_a = 0.1\tau_1^V T$ ,  $|\tau_{T_1}| = 16\tau_1^V T$ ,  $\tau_{T_2} = 130\tau_1^V T$ ,  $\tau_{D_1}^V = 16\tau_1^V T$  (for dipole molecules  $\tau_1^V T = 10^{-7}-10^{-3}$  sec, depending on the medium parameters). It is seen that even for  $t < \tau_D$  these processes affect substantially the variations in  $N'$ ,  $N_1'$ , and  $N_2'$ . Analysis shows that this effect is determined by the vibrational thermal diffusion, and is generated by the nonuniform distribution of the vibrational temperature  $T_1$  along the beam radius, which at  $t' = 1$  is  $\sim 4.5$  times larger than  $T_0$ , the variation in the translational temperature does not exceed in this case  $\sim 0.025 T_0$ , with the interaction parameter being  $\delta = 0.46$ . Thus, if in the model with  $k_V = 0$  we have  $N'(t) = N_1'(t) = N_2'(t)$  (only for  $t \sim \tau_D$  we have  $N_1' \neq N_2'$  due to the action of ordinary diffusion), for  $k_V = 1$  the shapes of the dependences  $N'(t)$ ,  $N_1'(t)$ , and  $N_2'(t)$  differ substantially. Since for small  $t$  the heating of the medium is not substantial, the decrease in  $\rho'$ , leading to a decrease in  $N_1'$ , is insignificant and the behavior of  $N_1'$  is primarily determined by the diffusion flow, generated in turn by the nonuniform distribution of  $T_1$ . For  $P_m = 0.5$  and  $P_N = 4$   $D_1^V < 0$ , the diffusion flow for molecules of a larger light gas A is directed from the periphery to the beam center, also leading to an increase in  $N_1'$  at the axis. For molecules of sort B the diffusion flow is directed from the center to the periphery ( $D_2^V > 0$ ), therefore  $N_2'$  decreases on the axis. For large  $t$  ( $t > 0.4\tau_D$ ) the variation in  $N_1'$  is already determined by the density variations along the beam axis. Therefore, reaching a maximum for some  $t$ , the  $N_1'$  value starts decreasing. The effect of macrotransport processes, related to excitation of molecular oscillations, on  $T'$  and  $T_1$  is substantially weaker. In this case the behavior of  $T_1$  is affected by not only the vibrational thermal diffusion, but also by the vibrational thermal conductivity, leading to a decrease in  $T_1$  on the beam axis in comparison with the model not including these processes ( $k_V = 0$ ). We note that for  $\zeta > 0$  (in the case being considered  $\zeta = -1$ ) one has kinetic cooling, and for  $\zeta < 0$  - kinetic warming of the medium [23].

The effect of the parameters  $\zeta$  and  $\theta_1$ , determined in terms of the spectroscopic characteristics of the absorption transition for  $P_a = 10$ ,  $P_I = P_D = 1$ ,  $P_m = 0.5$ ,  $P_N = 4$ , on the variations in  $N_1'$ ,  $N_2'$ ,  $T_3'$  (lines 1-3) with time on the beam axis is illustrated in Figs. 2 and 3 (in Fig. 2 the solid lines correspond to  $\theta_1 = 7$ , the dashed to  $\theta_1 = 3$ ,  $\zeta = -1$ , and in Fig. 3 the solid lines correspond to  $\zeta = -1$ , and the dashed to  $\zeta = -0.1$ ,  $\theta_1 = 3$ ). From the distributions presented it is seen that a decrease in  $\theta_1$  leads to smoother variation in all parameters and to an increase in the time of kinetic cooling. In this case the difference between the  $T'$  and  $T_1$  values, calculated by the complete model and by the model with  $k_V = 0$ , also increases. A decrease in  $|\zeta|$ , on the other hand, leads to a sharper variation in  $N_1'$ ,  $N_2'$ , and  $T'$ , and to a decrease in the time of kinetic cooling. Interesting here is the fact that the variation in  $\theta_1$  and  $\zeta$  changes substantially the behavior of the dependences  $N_1'(t)$ , though the parameters  $\theta_1$  and  $\zeta$  do not appear explicitly in the equations for  $N_1'$ . Their effect on  $N_1'$  occurs directly through the variation in  $T'$  and  $T_1$  [for decreasing  $\theta_1$   $T'$  and  $T_1$  vary more weakly, and for increasing  $\zeta$  ( $-1 \leq \zeta \leq 1$ ) - more strongly].

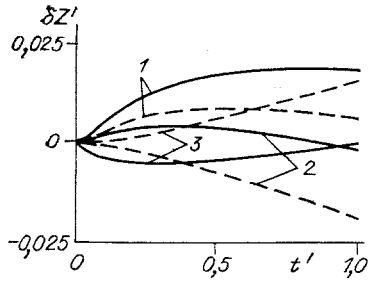


Fig. 3

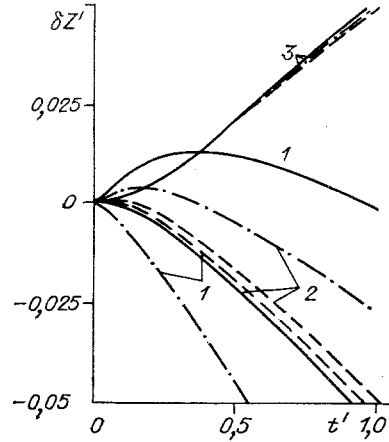


Fig. 4

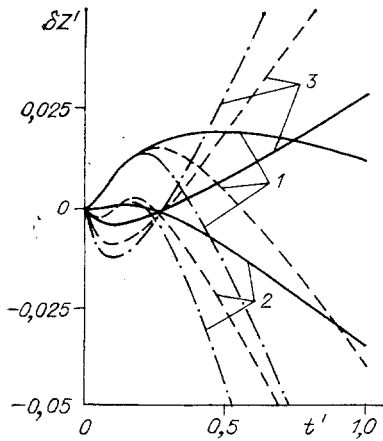


Fig. 5

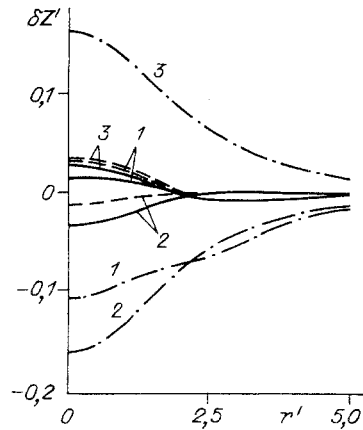


Fig. 6

The parameters  $P_m$  and  $P_N$  appear explicitly in the equations for  $N_1'$ ,  $N_2'$ ; besides, they determine the sign of  $k_T^i$ , and consequently, also the direction of the flow caused by both ordinary and vibrational thermal diffusion. Therefore, their effect on the variation of hydrodynamic parameters must be quite substantial. Figure 4 shows the dependences  $N_1'(t')$ ,  $N_2'(t')$ , and  $T'(t')$  (lines 1-3) at  $P_a = 10$ ,  $P_I = P_D = 1$ ,  $\theta_1 = 7$ ,  $\zeta = -0.1$ ,  $P_N = 4$  for  $P_m = 0.5, 1, 2$  (the solid, dashed, and dashed-dotted lines). It is seen that a variation of  $P_m$  from 0.5 to 2 leads to a qualitatively different behavior of  $N_1'(t')$ ,  $N_2'(t')$ . Thus, while for  $P_m = 0.5$  the function  $N_1'(t')$  has a maximum, and  $N_2'(t')$  decreases smoothly, at  $P_m = 2$  the situation is reversed. This is explained by the change in sign of  $k_T^i$ . The behavior of the dependences  $T'(t')$  is practically unchanged for different  $P_m$ . The effect of the parameter  $P_N$  is illustrated by Fig. 5, where lines 1-3 are provided for  $N_1'(t')$ ,  $N_2'(t')$ , and  $T'(t')$ , while the solid, dashed, and dash-dotted lines correspond to  $P_N = 4; 1; 0.25$  ( $P_m = 0.5$ ,  $P_a = 10$ ,  $P_I = P_D = 1$ ,  $\theta_1 = 7$ ,  $\zeta = -0.1$ ). It is seen that a decrease in  $P_N$  leads, firstly, to deeper cooling of the medium and its stronger subsequent heating, and, secondly, to sharper variations in  $N_1'(t')$  and  $N_2'(t')$ . The fact is interesting here that for  $P_N = 0.25$  the behavior of the dependences  $N_1'(t')$  and  $N_2'(t')$  is accurately determined by the behavior of  $T'(t')$  for small  $t'$ . As follows from (16)-(19), the changes in the relations between the characteristic times of processes must also affect the distribution of hydrodynamic parameters, both along the beam radius and in time. Lines 1-3 in Fig. 6 show the variations  $N_1'(r')$ ,  $N_2'(r')$ ,  $T'(r')$  at  $t = \tau_D$  for three characteristic cases, differing in the relations between  $P_a$ ,  $P_D$ ,  $P_I$ ,  $P_V$ : 1)  $P_a = 10$ ,  $P_V = P_I = P_D = 1$ ; 2)  $P_a = P_I = P_D = P_V = 1$ ; 3)  $P_a = P_I = P_V = 1$ ,  $P_D = 0.1$  (the solid, dashed, and dashed-dotted lines). The parameters  $\zeta$ ,  $\theta_1$ ,  $P_m$ ,  $P_N$  are identical ( $\zeta = -1$ ,  $\theta_1 = 7$ ,  $P_m = 0.5$ ,  $P_N = 4$ ). From the distributions presented it is seen that the relation between the VT-relaxation time and the diffusion time affects the variations in  $N_1'$ ,  $N_2'$ , and  $T'$  most strongly. A decrease in the ratio  $\tau_1^{VT}/\tau_D$  from 1 to

0.1 (a decrease in  $P_D$  from 1 to 0.1) leads to sharper heating of the medium, inducing a substantial decrease in  $N_1'$  (here  $N_1' < 0$ ) in comparison with the case  $P_V = P_D = 1$ , when  $N_1' > 0$ . Variations in the relation between  $P_a$  and the remaining parameters, characterizing the rates of various transport processes, affect the behavior of  $N_1'(r')$ ,  $N_2'(r')$ , and  $T'(r')$  to a lesser extent.

Thus, the analysis performed has shown that the excitation of molecular oscillations by resonance radiation with nonuniform intensity profiles along the beam radius leads to substantial enhancement in the effect of macrotransport processes on the variation of the hydrodynamic parameters of the medium. The laws of variation of these parameters are determined by the relations of characteristic times of the corresponding processes, the composition and masses of the mixture molecules, as well as the spectroscopic characteristics of the absorbing transition.

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COMPARISON OF MODELS WITH DIFFERENT AND IDENTICAL VIBRATIONAL TEMPERATURES OF MOLECULAR COMPONENTS

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UDC 533.6.011

During the entry of bodies into the Earth's atmosphere with a primary cosmic velocity the flow conditions at the fundamental thermal stress portion of designed trajectories are characterized by the absence of equilibrium between translational and vibrational degrees of freedom [1]. This result was obtained by using a model of one "averaged" vibrational temperature.

A model was considered in [2, 3], in which each molecular component corresponds to its vibrational temperature. These vibrational temperatures were found to differ insignificantly from each other, and the results practically coincide with calculation results using the "averaged" vibrational temperature. A number of simplifying assumptions were made in this case in [2, 3], including the neglect of the opposite effect of chemical reactions on vibrational relaxation, leading to a breakdown of the vibrational energy balance, resulting from not including its variations during generation and decay of molecules due to chemical reactions.

As shown in [1], with the development of dissociation the value of the corresponding source term is comparable with the value of the fundamental Landau-Teller term, and neglecting the effects mentioned above can lead to a substantial excess of the vibrational temperature over the translational one inside the shock layer, which was also observed in [2, 3].

In the present study we compare calculation results using an "averaged" model and different vibrational temperatures of molecular components for the example of flow in the vicinity of the critical line of the orbiting satellite "Buran."

1. Statement of the Problem. Consider stationary flow around an axially symmetric body due to a viscous chemically and thermodynamically nonequilibrium gas. We use the model of a thin viscous shock layer, being the asymptotic form of the Navier-Stokes equations for large Mach and Reynolds numbers, and density ratios before and after the shock wave, which is characteristic of the fundamental thermal stress portions of designed entry trajectories. Taking into account vibrational relaxation, the system of equations at the stagnation line can be written down as follows ( $y$  is the distance along the axis from the body):

$$\rho u + \frac{\partial}{\partial y}(\rho v) = 0, \quad \rho Du = -2p_1 + \frac{\partial}{\partial y} \left( \frac{\mu}{\text{Re}_\infty} \frac{\partial u}{\partial y} \right); \quad (1.1)$$

$$\frac{\partial p}{\partial y} = 0, \quad \frac{\partial p_1}{\partial y} = \rho u^2; \quad (1.2)$$

$$\rho c_p DT - \rho \sum_{k=1}^M DE_k^* - Dp = \frac{\partial}{\partial y} \left( \frac{\mu c_p}{\text{Re}_\infty \sigma} \frac{\partial T}{\partial y} + \sum_{k=1}^M q_k^v \right) - \sum_{i=1}^N h_i w_i - \left( \sum_{i=1}^N c_{vi} I_i \right) \frac{\partial T}{\partial y}; \quad (1.3)$$

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