

MUTUAL EFFECTS OF VIBRATIONAL-DISSOCIATIVE RELAXATION
 IN THE SUPERSONIC FLOW OF A VISCOUS GAS PAST BLUFF
 BODIES

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Along with the occurrence of nonequilibrium chemical reactions, the internal degrees of freedom of particles are excited during the motion of bodies at high supersonic velocities in the upper layers of the atmosphere. During re-entry along a glide path with an initial velocity $V_\infty \leq 8$ km/sec, neither ionization reactions nor electronic degrees of freedom make a significant contribution to the thermodynamics and state of the gas. However, vibrational relaxation is delayed due to the low density of the medium. Dissociation reactions, taking place against a thermodynamically nonequilibrium background (in the absence of thermal equilibrium between the translational and vibrational degrees of freedom), in turn affect the relaxation of vibrational degrees of freedom. Vibrational-dissociative interaction takes place.

A phenomenological model proposed in [1] included the effect of the relaxation of vibrations on chemical reactions. This effect was manifest in the appearance of correction factors in the rate constants for the dissociation reactions. The values of these factors depend on translational and vibrational temperature (CVD model). Treanor and Marrone of [2] made allowance for the effect of dissociation on vibrational relaxation (CVDV model) connected with the formation (recombination) and disappearance (dissociation) of molecules - carriers of vibrational energy. The CVDV model has been used mainly to study flows in the relaxation zone behind direct shock waves. As regards problems concerning the flow of a viscous gas past bodies, vibrational-dissociative interaction was considered in [3-5] within the framework of a model of a shock layer with a thin shock wave (SW). At the same time, simplified approaches have also been described in the literature. Afonina and Voronkin [6, 7] examined a model in which vibrational energy changes only due to V-T exchange described by the Landau-Teller term, and no allowance was made for the mutual effect of vibrational relaxation and dissociation. The calculations performed in [8-10] were conducted on the basis of the CVD model.

In the case of motion along a glide path, the effects of thermodynamic disequilibrium are manifest to the greatest extent in the diffuse shock wave regime. Thus, with allowance for the viscous shock wave, here we make use of simplified Navier-Stokes equations to compare the above-mentioned models and to demonstrate the effect of thermodynamic disequilibrium on flow characteristics. We will make use of the vibrational energy transport equation proposed in [11].

1. Formulation of the Problem. If effects associated with molecular transport in longitudinal (flight) directions are ignored, we have the following steady-state Navier-Stokes equations for a chemically and thermodynamically nonequilibrium gas

$$\frac{\partial}{\partial x^i} \left(\rho u^i \sqrt{\frac{g}{g_{(ii)}}} \right) = 0, \quad g_{33} = 1, \quad g_{3\alpha} = g_{\alpha 3} = 0; \quad (1.1)$$

$$\rho D u^\alpha + \rho A_{jh}^\alpha u^j u^h = - \sqrt{g_{(\alpha\alpha)}} g^{\alpha\beta} \frac{\partial P}{\partial x^\beta} + \sqrt{\frac{g_{(\alpha\alpha)}}{g}} \frac{\partial}{\partial x^3} \left(\frac{\mu \sqrt{g}}{\text{Re}_\infty} \frac{\partial u^\alpha}{\partial x^3} \right); \quad (1.2)$$

$$\rho D u^3 + \rho A_{jh}^3 u^j u^h = - \frac{\partial P}{\partial x^3} + \frac{4}{3} \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^3} \left(\frac{\mu \sqrt{g}}{\text{Re}_\infty} \frac{\partial u^3}{\partial x^3} \right); \quad (1.3)$$

$$\rho c_p DT = DP + \rho \sum_{k=M} c_k D\bar{e}_k + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^3} \left(\frac{\mu c_p \sqrt{g}}{Re_\infty \sigma} \frac{\partial T}{\partial x^3} - \frac{\sqrt{g}}{Re_\infty} \rho \sum_{k=M} c_k D_k \frac{\partial \bar{e}_k}{\partial x^3} \right) + \frac{\mu g_{\alpha\beta}}{Re_\infty} \frac{\partial u^\alpha / \sqrt{g_{(\alpha\alpha)}}}{\partial x^3} \frac{\partial u^\beta / \sqrt{g_{(\beta\beta)}}}{\partial x^3} + \quad (1.4)$$

$$+ \frac{4}{3} \frac{\mu}{Re_\infty} \left(\frac{\partial u^3}{\partial x^3} \right)^2 - \sum_{i=1}^N h_i \dot{w}_i - \left(\sum_{i=1}^N c_{pi} I_i \right) \frac{\partial T}{\partial x^3} + \sum_{k=M} \left(\dot{w}_k \bar{e}_k + I_k \frac{\partial \bar{e}_k}{\partial x^3} \right);$$

$$\rho \left(\sum_{k=M} c_k e'_k \right) DT_v + \left(\sum_{k=M} I_k e'_k \right) \frac{\partial T_v}{\partial x^3} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^3} \left[\frac{\sqrt{g}}{Re_\infty} \rho \left(\sum_{k=M} c_k D_k e'_k \right) \frac{\partial T_v}{\partial x^3} \right] + \quad (1.5)$$

$$+ \sum_{k=M} \left(c_{k0} \frac{e_k^0 - e_k}{\tau_k} - \dot{w}_k e_k + R_k \right);$$

$$\rho \dot{D}c_i + \frac{1}{\sqrt{g}} \frac{\partial \sqrt{g} I_i}{\partial x^3} = \dot{w}_i, \quad i = 1, \dots, N; \quad (1.6)$$

$$\frac{\mu}{Re_\infty} \frac{\partial m c_i}{\partial x^3} = \sum_{j=1}^N \frac{m^2}{m_j} S_{ij} (c_i I_j - c_j I_i); \quad (1.7)$$

$$P = R_G \rho \frac{T}{m}, \quad \sum_{i=1}^N I_i = 0, \quad \sum_{i=1}^N c_i = 1, \quad m = \left(\sum_{i=1}^N \frac{c_i}{m_i} \right)^{-1}, \quad (1.8)$$

$$c_p = \sum_{i=1}^N c_i c_{pi}, \quad D_k = \frac{\mu}{\rho} \sum_{i=1}^N (x_i S_{ik})^{-1}, \quad x_i = \frac{c_i m}{m_i},$$

$$\bar{e}_k = e_k^0 - e_k, \quad e_k^0 = \frac{R_G}{m_k} \frac{\theta_k}{\exp(\theta_k/T) - 1}, \quad e_k = \frac{R_G}{m_k} \frac{\theta_k}{\exp(\theta_k/T_v) - 1},$$

$$e'_k = \frac{\partial e_k}{\partial T_v}, \quad D = \frac{u^\alpha}{\sqrt{g_{(\alpha\alpha)}}} \frac{\partial}{\partial x^\alpha} + u^3 \frac{\partial}{\partial x^3},$$

$$A_{jk}^i = \frac{1}{2 \sqrt{g_{(jj)g_{(kk)}}}} \left[\sqrt{g_{(ii)}} g^{il} \left(\frac{\partial g_{kl}}{\partial x^j} + \frac{\partial g_{jl}}{\partial x^k} - \frac{\partial g_{jj}}{\partial x^l} \right) - \delta_j^i \frac{\partial \sqrt{g_{(jj)}}}{\partial x^k} - \delta_k^i \frac{\partial \sqrt{g_{(kk)}}}{\partial x^j} \right].$$

Here, summation is performed over identical indices; no summation is carried out over the indices in parentheses; unless otherwise noted, the English-letter indices take values of 1, 2, 3; the Greek-letter indices take values of 1, 2; $k = M$ denotes that summation is performed only for molecules; $g_{\alpha\beta}$ are components of the metric tensor; $V_\infty u^1$ are physical components of the velocity vector; T_0 and $T_v T_0$ are the translational and vibrational temperatures of a gas mixture consisting of N chemical species ($T_0 = V_\infty^2 / c_{p\infty}$); $c_{p\infty} T_0 e_k$, $T_0 \theta_k$ are the specific vibrational energy and the characteristic temperature of the k -th molecule; $V_\infty \tau_k / R$ is the relaxation time; $c_{p\infty} T_0 \rho_\infty V_\infty R_k / R$ is the source term. The rest of the notation is explained in [12].

The boundary conditions on the surface of the body, expressing the conditions of non-flow, attachment, and heterogeneous chemical reaction, and the heat-balance condition will be

$$x^3 = 0, \quad u^\alpha = u^3 = 0, \quad I_i = -\rho h_{wi} c_i, \quad i = 1, \dots, N,$$

$$q = \frac{\varepsilon \sigma_B T_0^4}{\rho_\infty V_\infty^3} T_w^4; \quad q = \frac{\mu c_p}{\sigma Re_\infty} \frac{\partial T}{\partial x^3} - \sum_{i=1}^N h_i I_i + \sum_{k=M} \left(\bar{e}_k I_k - \frac{\rho}{Re_\infty} c_k D_k \frac{\partial \bar{e}_k}{\partial x^3} \right).$$

For vibrational temperature, we assume that on the body

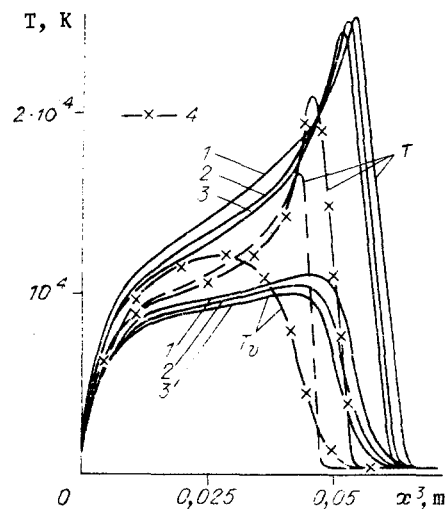


Fig. 1

$$T_v = T_w, \quad (1.9)$$

while in the case of a noncatalytic wall we also make use of the condition

$$\partial T_v / \partial x^3 = 0. \quad (1.10)$$

On the external boundary, we assign conditions corresponding to the parameters of the incoming flow.

In examining the chemical reactions taking place in the disturbed region of the flow, we take five species: N_2 , O_2 , N , O , and NO . Dissociation-recombination reactions and exchange reactions take place between these components of the mixture.

Since the characteristic vibrational temperatures for the molecules of partly dissociated air differ from one another by a factor of no more than 1.5, we will take a certain mean temperature in Eqs. (1.1)-(1.8). This mean temperature will be the same for all of the molecules. Equation (1.4) is written in a form in which the terms connected with relaxation of vibrational degrees of freedom are explicitly expressed. These terms vanish with the approach toward thermodynamic equilibrium $\bar{e}_k \rightarrow 0$ and the heat-flux equation (1.4) takes the usual form in which the vibrational degrees of freedom are in equilibrium with the translational degrees of freedom. The enthalpies and heat capacities of the species in (1.4) should be calculated with thermodynamic equilibrium. We took their values from the tables in [13], where the equilibrium state with respect to electronic degrees of freedom was also taken into account. Equation (1.5) is the result of the summation of the vibrational energy balance equations of the molecules with the assumption that their vibrational temperatures are equal.

The effect of vibrational relaxation on the dissociation reactions is manifest in a change in the rate constants for these reactions

$$k_D(T, T_v) = k_D(T)V(T, T_v),$$

where $k_D(T)$ is the dissociation constant under thermodynamic equilibrium, when $T_v = T$; $V(T, T_v)$ is a function whose explicit form depends on the probability assigned in the CVD model for the transition of molecules from vibration levels v in the continuous spectrum. In the present study, we took this probability to be equal to [14]

$$F(v) = \exp[-(E_D - E_v)/kU]$$

(E_D and E_v are the dissociation energy and the energy of the level v ; U is a parameter having the dimension of temperature and determining the degree of preferential dissociation from the upper levels compared to the lower levels). The reverse effect of the chemical reactions on vibrational relaxation is accounted for through the source term R_k within the framework of the CVDV model [2]. The vibrational relaxation time was calculated from the Milliken-

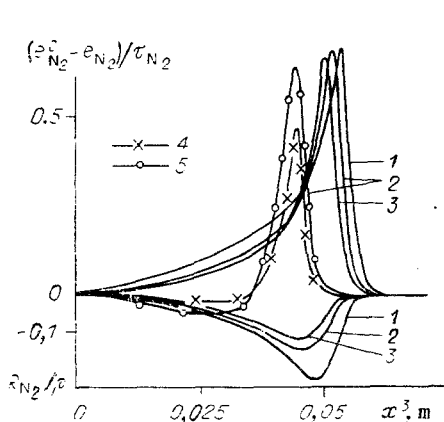


Fig. 2

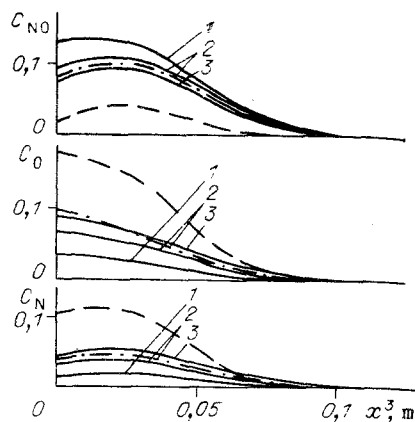


Fig. 3

White formula for gas mixtures with the correction for high temperatures proposed in [9]. The method used to solve the problem numerically was similar to that described in [12, 15].

2. Analysis of the Results. Presented below are the results of calculations performed for a body with radii of principal curvature 0.5 and 1.25 m and $\epsilon = 0.85$. The conditions in the incoming flow correspond to motion along the glide path from [16]. The following values of the characteristic temperatures and dissociation temperatures were assigned for molecules of N_2 , O_2 , and NO : $\theta_i = 3372, 2256, 2720$ K; $T_{Di} = 113\,000, 59\,500, 75\,500$ K.

Figure 1 shows profiles of translational and vibrational temperatures on the critical line for an ideally catalytic surface at $H = 75$ km ($Re_\infty = 6.95 \cdot 10^3$). Here and below, we used the following notation: the solid lines represent calculations performed by the CVDV model with boundary condition (1.9) for vibrational temperature; the dashed lines show the results of calculations of a thermodynamically equilibrium flow past the body, i.e., with the assumption that the vibrational temperature coincides with the translational temperature. Numbers 1-3 correspond to the values $T_D/U = 6; 3; 2$.

Allowing for vibrational relaxation leads to a substantial increase in translational temperature. An increase in the probability of the dissociation of molecules from upper vibration levels (a decrease in the parameter U) is accompanied by an increase in vibrational and translation temperature and the size of the disturbed region of the flow. These events are in turn associated with a decrease in density in the shock layer, but the pressure on the body at the critical point decreases by no more than 2%. Due to the presence of a relaxation zone in the leading edge of the shock wave, the flow undergoes a smoother deceleration (with smaller gradients) than in the thermodynamically equilibrium case.

For the same conditions as above, Fig. 2 shows profiles of the source of vibrational energy due to V-T exchange (Landau-Teller term) and the source of vibrational energy R_{N_2}/ρ due to reactions. The choice of a model in which the molecules undergo a transition from a discrete spectrum to a continuous spectrum has little effect on the maximum value of the source of vibrational energy due to V-T exchange. The parameter U is substantial for the profile of the source R_k/ρ , which is responsible for the reverse effect of dissociation on vibrational relaxation.

We will examine certain simplified models that allow for internal degrees of freedom and that have been used previously in the literature for problems involving external flow past a body. Lines 4 in Figs. 1 and 2 correspond to a model in which vibrational energy changes only due to the Landau-Teller term. No allowance is made for vibrational-dissociative interaction. In this case, the correction factors V are assumed to be equal to unity and the term $\sum_{k=M} R_k$ is absent from Eq. (1.5). Line 5 in Fig. 2 corresponds to a CVD model in which allowance is made for the effect of vibrations on the rate of the chemical reactions, but the reverse effect of dissociation on vibrational energy (the term $\sum_{k=M} R_k$) is ignored. Both models lead in the case of developed dissociation to a physically unrealistic situation whereby the vibrational temperature exceeds the translational temperature inside the shock layer (the region of negative values of the Landau-Teller term). When the CVDV model is used

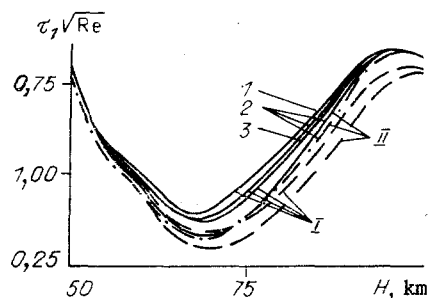


Fig. 4

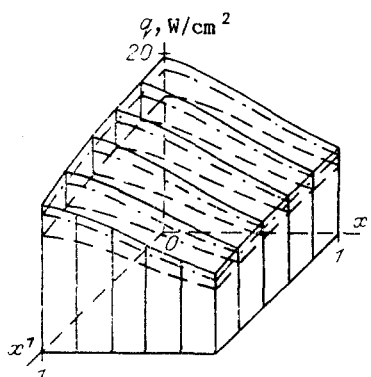


Fig. 5

with boundary condition (1.9) for the wall, the calculated vibrational temperature does not exceed the translational value. It follows from Fig. 2 that, with developed dissociation, ignoring the effect of chemical reactions on vibration leads to the discarding of terms which are equal in order of magnitude to the Landau-Teller terms. This error increases with a decrease in U .

Figure 3 shows profiles of concentration on the critical line for a noncatalytic surface with $H = 90$ km ($Re_\infty = 845$). Here and below, the dot-dash lines correspond to calculations performed in accordance with the CVDV model with boundary condition (1.10) for vibrational temperature. It was found in the calculations that dissociation begins against a thermodynamically nonequilibrium background over almost the entire glide path. The effect of the vibrational degrees of freedom on dissociation leads to a reduction in the rate of dissociation due to a deficit of highly excited and, thus, readily dissociated molecules. The presence of thermodynamic disequilibrium leads to an increase in translational temperature and, thus, the equilibrium rate constant of the dissociation reactions k_p . However, the factor V — equal to the ratio of the actual dissociation constant to the equilibrium value — decreases to a value considerably less than unity due to the difference between the vibrational and translational temperatures. Thus, the rate of formation of atoms decreases.

The correction factor $V \ll 1$ in the upper part of the trajectory, where there is a very large difference between the vibrational and translational temperatures. This leads to strong suppression of dissociation, and the concentration of atoms decreases several-fold. With a decrease in flight altitude and approach of the profiles of vibrational and translational temperature, V increases and the reduction in the degree of dissociation becomes smaller. Allowance for vibrational disequilibrium increases the content of molecules of nitric oxide in the shock layer. This event is related to the fact that the relaxation of the vibrations has no effect on recombination reaction, while the rate of the dissociation of nitric oxide decreases due to the effect of vibrations.

A reduction in U suppresses dissociation. The parameter U , characterizing the degree of the reduction in the probability of dissociation from lower vibration levels, reflects the uncertainty over the specific mechanism responsible for dissociation and must be found from an experiment. Canac and Vaughan [17] used the value $U_{O_2} = T_{DO_2}/6$, which corresponds to a 300-fold increase in the level of probability of the transition of O_2 molecules to the continuous spectrum from the upper vibration levels compared to the same probability from lower levels. The value $U = T_D/2$ corresponds to a situation in which the first probability is seven times greater than the second probability. The actual value of U evidently lies within the range $T_D/6 \leq U \leq T_D/2$.

The use of a model in which the change in vibrational energy is due only to the Landau-Teller term and $V = 1$ leads to an increase in the rate of the dissociation reactions due to an increase in translational temperature. As a result, the concentration of atoms increases while the content of nitric oxide molecules decreases compared to the thermodynamically equilibrium case.

Figure 4 shows the effect of thermodynamic disequilibrium at the critical point on the value of the dimensionless friction coefficient τ/Re calculated from the formula $\tau_1 = \tau/x^1$, $\text{Re} = \rho_\infty V_\infty R/\mu(T_0)$. Lines I correspond to an ideally catalytic surface, while lines II correspond to a noncatalytic surface. Allowance for the relaxation of vibrational degrees of freedom increases the friction coefficients by up to 5-10%.

Figure 5 shows the distribution of heat flux along the lateral surface of an elliptical paraboloid for a noncatalytic surface with $H = 95$ km ($\text{Re}_\infty = 415$). Allowance for vibrational relaxation with boundary condition (1.9) leads to an increase in heat flux for the entire glide path. For a wall with boundary condition (1.10) at altitudes where intensive recombination occurs, the heat flux may be lower than in calculations performed with the assumption of equilibrium excitation of internal degrees of freedom. Vibrational relaxation has a strong effect on relative heat flux in the upper part of the trajectory. It should be noted that, in this part (at $H \geq 90$ km), it is important to make allowance for processes occurring in the Knudsen layer around the body. Here, it is necessary to use boundary conditions accounting for slip on the body in order to expand the range of validity of the continuum model.

In conclusions, we note that the solution of external flow problems by means of the model which accounts only for V-T exchange (Landau-Teller term) or the CVD model may lead to an unjustified increase in vibrational temperature over translational temperature. In the case of developed dissociation, ignoring the reverse effect of chemical reactions on vibration leads to the rejection of terms which are of the same order of magnitude as the corresponding Landau-Teller relaxation terms. This error increases with a decrease in the parameter U , characterizing the probability of dissociation from different vibration levels. Thus, allowance for the mutual effect of vibrational relaxation and chemical reactions is necessary for correct qualitative and quantitative modeling of supersonic flows with physicochemical changes occurring in regimes in which vibrational relaxation time becomes commensurate with the time of occurrence of dissociation reactions.

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RELAXATIONAL PROPERTIES OF A TURBULENT SHEAR FLOW ACROSS
A CYLINDER IN THE PRESENCE OF A PLATE

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With the use of semi-empirical turbulence models to analyze essentially nonequilibrium turbulent boundary layers in the last decade, there have been increasingly frequent complaints about the inadequacy of the traditional approaches that have been employed to solve such problems [1]. One reason for this dissatisfaction is the local nature of the turbulence hypotheses for the external region, which is characterized by the presence of large, long-lived eddies - the main sources of information on perturbations. In connection with this, the Boussinesq approximation proves to be inadequate for the analysis of flows in this region. As regards the internal region - characterized by small-scale turbulence and offering less information on perturbations - the use of the Boussinesq hypothesis is obviously valid. This shows the need to resort to the use of a relaxation theory (heredity theory) based on a new formula for turbulent shear stress that will make it possible to account for the history (memory) of the boundary layer in regard to a given disturbance. By relaxation, in the process by which some physical quantity derived from the equilibrium state returns to this state [2].

The first attempt to account for relaxation processes in turbulent shear flows was made by Hinze [3] by means of an equation that was also derived and analyzed in detail in [2]. The equation is based on a generalization of the Maxwell model to the case of turbulent motion:

$$L_x^* \overline{\partial u'v'} / \partial x + L_y^* \overline{\partial u'v'} / \partial y + \overline{u'v'} = -\nu_t \overline{\partial u} / \partial y, \quad (1)$$

where L_x^* and L_y^* are the longitudinal and transverse relaxation paths, having the dimension of length; $\overline{u'v'}$ is the turbulent shear stress; \bar{u} is velocity; ν_t is eddy viscosity; the superimposed bar denotes averaging over time.

In the solution of the relaxation equation, the quantities L_x^* and L_y^* are preassigned functions of the longitudinal coordinate x and transverse coordinate y even in the case of two-dimensional nongradient flow. However, this question has yet to be fully resolved, since the amount of reliable data now available on the laws governing the change in relaxation length is clearly inadequate. There is also no systematic data on the effect of the form of the source of perturbations and its relative dimensions on relaxation processes in shear flows. On the other hand, the study of the structure of a flow past different types of projections, irregularities, and obstacles is of interest in its own right - especially from the viewpoint of solving a whole range of practical problems [4, 5]. Thus, the tendency seen in recent years to account for relaxation phenomena in the analysis of nonequilibrium turbulent boundary layers requires more intensive study of the hydrodynamic structure of shear flows beyond perturbation sources of different geometries. Also required in this connection is determination of the laws which govern the change in the characteristic relaxation lengths under given conditions.

In the present study, we analyze the possibility of using the Hinze relaxation equation for a nonequilibrium turbulent shear flow which develops after the fluid crosses a circular

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