

## LITERATURE CITED

1. N. I. Melik-Pashaev, É. K. Moroz, and A. I. Mel'nikov, *Inzh.-Fiz. Zh.*, **58**, No. 2, 197-199 (1990).

### EFFECT OF THE DISSOCIATION MODEL ON CALCULATIONS OF HEAT EXCHANGE DURING SMOOTH DESCENT

V. G. Shcherbak

UDC 533.6.011

*The effect is demonstrated of the choice of a model for dissociation on the results of calculating the flow characteristics near a body, in the absence of equilibrium between the translational and vibrational degrees of freedom.*

The flow in a shock layer near a body which is moving along a smooth re-entry trajectory into the Earth's atmosphere for  $H \geq 50$  km is characterized by high temperatures ( $10^3 \leq T \leq 2 \cdot 10^4$  K) and the absence of equilibrium between the translational and vibrational degrees of freedom [1]. Under such conditions, the rate constant for dissociation will be determined not only by the translational temperature (as is assumed in the majority of systems in the literature of data on the chemical reaction constants), but on the vibrational temperature as well. It will also depend on the relative probability of dissociation from various vibrational levels and on other factors. For this reason, the experimental values of the dissociation rate constants found in the literature differ by several orders of magnitude in the high temperature region. The problem is that the experiments are performed under various conditions (differing in pressure), and consequently, for different values of the vibrational temperature. The latter is not figured along with the translational temperature as a determining parameter when presenting results on reaction rates.

For reasonable physical assumptions (the collisional cross section does not depend on the vibrational level of the colliding particles or their relative velocity, the chemical reaction does not violate a Maxwellian velocity distribution, populations of levels are quasi-Boltzmann), the total dissociation constant can be represented in the form

$$K(T, T_v) = K^0(T) V(T, T_v),$$

where  $K^0(T)$  is the equilibrium dissociation rate constant (for  $T_v = T$ ), and  $V$  is a function whose form depends on the dissociation model adopted. Various dissociation models have been proposed in the literature, which are used to interpret experimental data from shock tubes. Vibrational relaxation must be taken into account when processing experimental data on the chemical reaction rate constants in air.

Such work was carried out in [2] on the basis of the dissociation model in [3], and the equilibrium part of the dissociation constant  $K^0(T)$  was separated out. In addition, an approximation of the total dissociation constant  $K$  depending only on the translational temperature was also proposed in [2].

In this paper, the results obtained with the use of this approximation are compared to the results of calculations which take into account vibrational relaxation on the basis of  $K^0(T)$ , with the application of dissociation models from [3-7]. The

calculations were done for the flow in the neighborhood of the critical line of the orbital vehicle "Buran" during its motion along a re-entry trajectory.

According to the model of single-temperature kinetics, the reaction rate constants depend only on the temperature of the translational degrees of freedom and dissociation takes place primarily from the higher vibrational levels. This classical model of dissociation is groundlessly extrapolated to high temperatures ( $T \geq 8 \cdot 10^3$  K), since it is experimentally verified for low temperatures in the presence of an established equilibrium between the translational and vibrational degrees of freedom. According to this dissociation model, the molecules execute a "climb up the staircase of vibrational states," from low levels to higher ones, and are then found in the interval  $kT$  near the dissociation limit. Subsequent collisions then result in dissociation. Various dissociation models have been proposed in the absence of equilibrium between the translational and vibrational degrees of freedom. Let us examine these models.

*Model 1.* Dissociation does not violate a Boltzmann distribution, and takes place by means of the transfer of molecules with effective vibrational levels which are located within the quantity  $\beta kT$  of the dissociation limit [3]. The function  $V$  has the form:

$$V(T, T_v) = \frac{Z(T)}{Z(T_v)} \exp \left[ - \frac{D - \beta kT}{k} \left( \frac{1}{T_v} - \frac{1}{T} \right) \right].$$

For the truncated harmonic oscillator model, these levels are expressed in the following way:

$$Z_h(T_v) = [1 - \exp(-\theta/T_v)]^{-1}.$$

In experiments investigating nonequilibrium dissociation in shock tubes, the values  $\beta = 3$  for  $N_2$  and  $NO$ , and  $\beta = 1.5$  for  $O_2$  have been obtained.

*Model 2.* Dissociation takes place with definite probabilities from any vibrational state and does not violate the distribution of molecules by vibrational level. The distribution of the probability is assumed to be exponential with a single fit parameter  $U$ , having the dimension of temperature and determining the degree of predominance of dissociation from the upper levels in comparison with the lower [4]:

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

where  $E_v$  is the energy level.

Assuming a Boltzmann distribution with temperature  $T_v$ , the function  $v$  has the following form:

$$V(T, T_v) = \frac{Z(T) Z(T_F)}{Z(T_v) Z(-U)} \frac{1}{T_F} = \frac{1}{T_v} - \frac{1}{T} - \frac{1}{U}.$$

In [4] it was assumed that  $U = D/kg$ , where  $g = 6$ .

*Model 3.* Experimental results from [5] showed that  $g \sim T^{-1}$ , and it was proposed that  $U = T/1.7$  be adopted.

*Model 4.* In [6], it was proposed that the reaction rate of dissociation be described by formulas obtained using the assumption of thermodynamic equilibrium, but with the replacement of the argument  $T$  by  $T_v$ . For example, if the rate constant is given by an Arrhenius formula, then

$$K = AT_*^n \exp(-E/kT_*), \quad T_* = T_v,$$

where  $A$ ,  $n$ ,  $E$  are a pre-exponential factor, the power index, and the activation energy, known for the chemical kinetics for  $T_* = T$ .

*Model 5.* In [7], it was proposed that the argument  $T$  in the formula for the reaction rate constant of dissociation be replaced by an "averaged" temperature  $T_* = \sqrt{TT_v}$ , which to some degree accounts for the deviation of  $T_v$  from  $T$ .

We further examine flow past bodies during their motion along a planned re-entry trajectory into the Earth's atmosphere. The system of equations of a hypersonic viscous shock layer in the neighborhood of the critical line were given in [1]. These equations take into account nonequilibrium chemical reactions, multicomponent diffusion, and vibrational relaxation. Five components were assumed to be present in the shock layer;  $N_2$ ,  $O_2$ ,  $NO$ ,  $N$ , and  $O$ , between which dissociation, recombination, and exchange reactions take place. For the vibrational temperature at the surface, it was assumed that

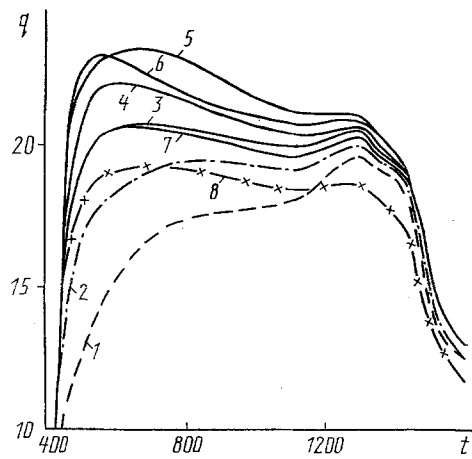


Fig. 1. Heat flux as a function of descent time: 1, 2) neglecting vibrational relaxation, for  $K^0(T)$  and  $K(T)$  from [2]; 3-7) taking vibrational relaxation into account, for dissociation models in [3-7], and boundary condition (1); 8) dissociation model from [3] and boundary condition (2).  $q$ ,  $10^4$  W/m<sup>2</sup>;  $t$ , sec.

the conditions of equilibrium were satisfied, or that the walls were noncatalytic with respect to the internal degrees of freedom:

$$T_v = T_w, \quad (1)$$

$$\partial T_v / \partial y = 0. \quad (2)$$

Note that models 4 and 5 are based only on general considerations of the role of vibrational excitation in the chemical reaction kinetics. When computing source terms responsible for the reverse effect of the chemical reactions on vibrational relaxation, one must know the average change in the vibrational energy for one dissociation and recombination event. Their values for models 4 and 5 are computed according to the expressions which follow from model 1.

Figure 1 shows the values of the thermal flux at the critical point on the orbital vehicle "Buran" as a function of descent time, during its motion along a smooth re-entry trajectory [8]. The radius of the truncated nose is 0.83 m, the albedo of the surface is 0.8, and the surface of the body is assumed to be noncatalytic with respect to heterogeneous recombination reactions. The section of the trajectory shown covers the range of heights  $H = 100$ -52 km.

The calculations shown by curves 1, 2 satisfy the assumption that all internal degrees of freedom are excited in equilibrium, with the use of the corresponding constants  $K^0(T)$  and  $K(T)$  from [2]. Curves 3-7 correspond to the results of calculations which take into account vibrational relaxation on the basis of the equilibrium constant  $K^0(T)$  and dissociation models from [3-7], with boundary condition (1). Curve 8 was calculated using dissociation model from [3] and boundary condition (2) for the vibrational temperature. The difference between the results denoted by curve 1 and curves 3-8 indicates the influence of nonequilibrium excitation of vibrational degrees of freedom.

Dissociation constants  $K(T)$  were proposed in [2] as approximations to the experimental data based only on the translational temperature.  $K^0(T)$  was obtained in [2] by manipulating the results in accordance with the model from [3]. The heat fluxes calculated on their basis differ from one another (curves 2 and 3, 8).

The use of different dissociation models leads to different results (curves 3-7). These results can differ by 15% in the values of the heat flux and by 50 K in the equilibrium temperature of the surface.

Boundary conditions (1) and (2) are limiting cases which describe the interaction of the surface of the body with the vibrational degrees of freedom. For the dissociation model of [3], the values of the unknown quantities for realistic surface

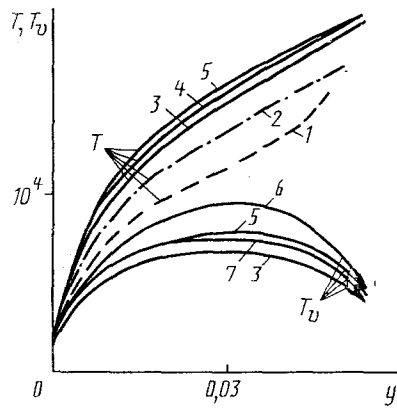


Fig. 2. Profiles of translational and vibrational temperature at  $t = 540$  sec. Notation as in Fig. 1.  $T$ , K;  $y$ , m.

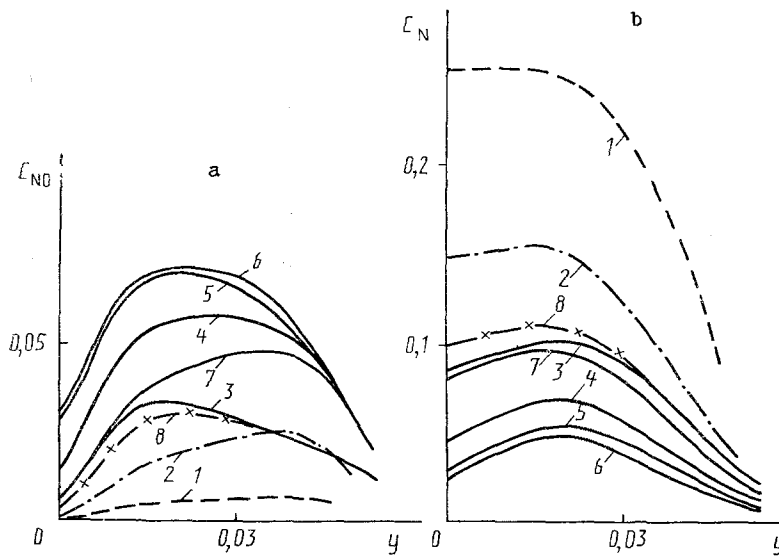


Fig. 3. Profiles of mass concentration of NO molecules (a) and N atoms (b). Notation as in Fig. 1.

properties are evidently found within the limits of the results obtained (curves 3 and 8). For the trajectories examined, this range consists of up to 10% by heat flux and up to 35 K by surface temperature.

Figure 2 shows profiles of the translational and vibrational temperatures for  $t = 540$  sec ( $H = 86.2$  km,  $V_\infty = 7.575$  km/sec). The relative positions of the profiles for the different models is the same for other points on the trajectory.

The profiles of the translational temperature, computed using models [3] and [7] are close to one another. The same is true for models [5] and [6]. For models [5] and [4], the vibrational temperatures are near one another. For calculations along the trajectory using the different models, the difference in the values can reach 2000 K for the translational temperature, and up to 2500 K for the vibrational temperature, inside the shock layer. After passage of the shock wave, the influence of the various dissociation models is insignificant.

Figure 3, which shows the mass concentration profiles for NO molecules and atomic N at the same point on the trajectory, illustrates the sensitive dependence of the composition of the air in the shock layer on the dissociation model.

The results given here show quantitatively and qualitatively the dependence of the characteristics of the flow on the dissociation model chosen. To correctly model flow characterized by high temperatures, it is necessary to refine the dissociation model and to take vibrational relaxation into account when processing experimental data on the reaction rate constants for dissociation.

The approximation of the total constant of dissociation as a function of only the translational temperature cannot be extended to a change in flow regimes for motion of bodies along a smooth re-entry trajectory.

## NOTATION

$T$ ,  $T_v$ , translational and vibrational temperatures;  $K^0$ ,  $K$ , equilibrium and total dissociation rate constants;  $D$ , energy of dissociation;  $k$ , Boltzmann constant;  $Z$ , statistical sum of the vibrational levels;  $\theta$  characteristic temperature of the molecules;  $T_w$ , equilibrium temperature of the surface;  $q$ , heat flux;  $t$ , descent time;  $H$ , height;  $V_\infty$  flight velocity;  $y$ , distance from the body along the normal.

## LITERATURE CITED

1. A. G. Tirskii, V. S. Shchelin, and V. G. Shcherbak, *Mat. Modelirov.*, **2**, No. 4, 28-38 (1990).
2. O. É. Krivonosova, S. A. Losev, V. P. Nalivaiko, et al., *Khim. Plazmy*, No. 14, 3-31 (1987).
3. S. A. Losev and N. A. Generalov, *Dokl. Akad. Nauk SSSR*, **141**, No. 5, 1072-1075 (1961).
4. P. V. Marrone and C. E. Treanor, *Phys. Fluids*, **6**, No. 9, 1215-1221 (1963).
5. B. V. Kuksenko and S. A. Losev, *Dokl. Akad. Nauk SSSR*, **185**, No. 1, 69-72 (1969).
6. K. L. Wray, E. V. Feldman, and P. F. Lewis, *J. Chem. Phys.*, **53**, No. 11, 4131-4136 (1970).
7. C. Park, "Assessment of a two-temperature kinetic model for dissociating and weakly-ionizing nitrogen," AIAA paper No. 1347, New York, (1986).
8. G. E. Lozino-Lozinskii, *The Gagarin Scientific Lecture Series on Cosmonautics and Aviation 1989* [in Russian], Moscow (1990), pp. 6-21.

## INFLUENCE OF THERMAL EFFECTS ON THE PROCESS OF HIGH-VELOCITY PENETRATION OF A FLUORO-POLYMER PLATE

V. A. Gorel'skii and S. A. Zelepugin

UDC 539.537

*We examine the problem of high-velocity impact of a steel cylinder on a fluoro-polymer plate. The finite-element numerical method is used to study the distributions of thermal and mechanical variables which result from the process of this axisymmetric interaction. The features of plate penetration are revealed when the temperature in some regions of the fluoro-polymer exceed melt, and thermal dissociation takes place.*

*Introduction.* The broad application of polymer materials in technology has made the study of their behavior under extreme conditions, particularly under shock-wave loading, topical [1]. Certain aspects of the behavior of polymers under high-velocity impact conditions have already been reflected in the experimental works of [2, 3], where the effects of heating on the strength properties of polymers was shown.

However, numerical calculations are needed to determine the dynamics of the temperature field distribution which arises in the penetration process, and to evaluate the influence of this field on the mechanical characteristics of the material. The goal

---

Institute of Structural Macrokinetics, Tomsk Branch, Russian Academy of Sciences, Tomsk. Translated from *Inzhenerno-Fizicheskii Zhurnal*, Vol. 62, No. 4, pp. 564-568, April, 1992. Original article submitted August 2, 1991.