Journal of Applied Mechanics and Technical Physics, Vol. 43, No. 5, pp. 649–653, 2002

CALCULATION OF IONIZATION AND RADIATIVE CHARACTERISTICS OF AIR IN THE SHOCK LAYER ON THE BASIS OF VARIOUS MODELS OF VIBRATION–DISSOCIATION INTERACTION

S. V. Shilenkov

UDC 533.6.011

Models of vibration-dissociation interaction are verified on the basis of results of numerical simulation of nonequilibrium air flow in the shock layer near vehicles flying in the atmosphere and data of in-flight and wind-tunnel experiments on measurement of ionization and radiative characteristics of the shock layer.

Introduction. An important element of numerical simulation of nonequilibrium flows in a viscous shock layer near a vehicle flying in the atmosphere is the choice of the model of physicochemical transformations. The model should describe the main processes in the high-temperature shock layer, which affect gas-thermodynamic and kinetic characteristics of the flow. The fact that there exist many models (which are often contradictory) for each physicochemical process hinders the mathematical description of the flow.

Assumptions made in creating the model of a physical process are often invalid under conditions of a real flight. Interaction of various physicochemical processes in nonequilibrium flows can also be so intense that the error in one of them can affect practically all flow parameters. This is completely true for the vibration-dissociation interaction (VDI). A large number of models of this process are currently known. Formally, they can be classified into three groups.

1. Empirical models (for instance, Park's model [1]), which do not contain theoretical assumptions on the VDI structure. Calculations by these models yield only a lower dissociation rate at low vibrational temperatures. In Park's model, this is achieved by averaging the translational and vibrational temperatures with the use of various values of the empirical exponent s, which allows one to adapt the model to various flight conditions being simulated.

2. Semi-empirical models, which include the β-model [2] based on the assumption that the molecules start to dissociate from a certain vibrational level D–βkT (D is the energy of dissociation, k is the Boltzmann constant, and T is the translational temperature; the parameter β is determined experimentally for each molecule under study; it equals 1.5 and 3 for oxygen and nitrogen molecules, respectively).

3. Models that do not contain empirical parameters and are completely theoretical (for instance, Kuznetsov's model [3]).

Despite the large number of VDI models, the validity of using some of them in numerical simulation of parameters of nonequilibrium flow of a reacting mixture of gases cannot be evaluated *a priori*.

At the same time, in determining ionization parameters of the viscous shock layer near the vehicle at the atmospheric flight trajectory, one needs not only a correct description of the process of nonequilibrium ionization or reaction with participation of electrons and ions but also correct temperatures and concentrations of neutral components of the gas, since the variation in these parameters leads to a significant variation in electron and ion concentrations. Thus, nonequilibrium ionization is extremely sensitive to the choice of the VDI model. The above information on nonequilibrium ionization refers also to spectral-energy characteristics of nonequilibrium radiation in band systems of the NO molecule. This is related to the dependence of concentrations of electron-excited states of the nitric oxide molecule, which determine nonequilibrium radiation in band systems of NO molecules, on

Central Aerohydrodynamic Institute, Zhukovskii 140180. Translated from Prikladnaya Mekhanika i Tekhnicheskaya Fizika, Vol. 43, No. 5, pp. 13–19, September–October, 2002. Original article submitted January 10, 2002; revision submitted March 14, 2002.

0021-8944/02/4305-0649 $27.00

temperatures and concentrations of nitrogen and oxygen atoms, which are determined, in particular, by the choice of the VDI model. In view of the existing uncertainty in the choice of the model of the process, one has to compare the numerical data obtained on the basis of various models with the results of wind-tunnel or in-flight experiments. In particular, this approach was used in [4, 5] in developing models of the formation of nonequilibrium radiation in the shock layer near space vehicles flying in the Earth [4] and Mars [5] atmospheres.

In the present work, verification of VDI models is performed by comparing ionization and radiation characteristics of the flow, which were obtained by numerical simulation, with the data of in-flight experiments performed at various times in the U.S.A. The objective of these experiments was the measurement of ionization and radiation parameters of the flow in the shock layer, aimed at the development of mathematical and physical models of the flow around space vehicles. In particular, in the flight of the "Bow Shock-2" spacecraft [6], the measured intensity of shock-layer radiation was within the spectral range of (230 ± 25) nm, which corresponds to radiation in band systems of nitric oxide molecules. A detailed study of nonequilibrium ionization in the shock-layer region was performed in flights of the RAM spacecraft series [7]. The electron concentrations across the shock layer were measured, which allowed one to verify the ionization model in numerical programs for simulation of the nonequilibrium flow around vehicles in the Earth atmosphere.

Along with the in-flight data, for additional verification of the physical model, we use the results of a wind-tunnel experiment on nonequilibrium ionization and radiation characteristics of the flow behind a strong shock wave in air, which were obtained in an electric-discharge shock tube of the Central Aerohydrodynamic Institute.

Numerical Simulation of a Nonequilibrium Air Flow in the Shock Layer. In numerical simulation of a nonequilibrium flow in the shock layer near a spacecraft flying in the Earth atmosphere, we used a set of programs implementing numerical and physical models based on the full Navier–Stokes equations, which were described in detail in [4].

In the kinetic model, we take into account the multispecies gas in the shock layer, which is a mixture of molecules (N_2, O_2, and NO), atoms (N and O), ions (NO^+, N_2^+, and O_2^+), and electrons, the difference between the temperatures of translational (T) and vibrational degrees of freedom of the N_2, NO, and O_2 molecules (T_{vN_2}, T_{vNO}, and T_{vO_2}, respectively), dissociation (recombination) of N_2, NO, and O_2 molecules, exchange processes with the formation of NO molecules, vibration-dissociation interaction, and reactions of ionization including associative ionization (reactions of the formation of NO^+, N_2^+, and O_2^+ ions and electrons) and charge exchange between ionized and neutral atoms and molecules of the mixture.

In calculating the characteristics of radiation of the shock layer near the spacecraft, we take into account the nonequilibrium character of radiation formation in most intense band systems of molecules under flight conditions [ultraviolet range: NO(β), NO(δ), NO(ε), and NO(γ)]. In numerical simulation of radiation processes, we use the multilevel model of population (destruction) of electron-vibrational radiative states of molecules, where their concentration is determined by solving the "balance" differential equations that describe the processes of resonance exchange of excitation energy between different components, collisional processes with participation of heavy particles and electrons, reactions of dissociation and recombination, and also radiative depletion of these states. The physical model of these processes was considered in more detail in [4], where the rate constants were also given.

The intensity of nonequilibrium radiation of the shock layer was calculated for all examined systems of molecular bands on the basis of a database of spectroscopic constants and Einstein's coefficients for electron-vibrational transitions, which was developed in [8]. In the present work, we have not considered atomic radiation and radiation in free–free and free–connected transitions, since these processes play an insignificant role in the overall radiative balance for flight velocities $V_\infty \leqslant 7$ km/sec.

The following VDI models were considered in the present work:

1. Park's model [1]. The empirical parameter s was first assumed to be equal to 0.5; later on, it was recommended to use the value $s = 0.7$, which is in better agreement with the results of numerical simulation of the processes of vibrational excitation and dissociation.

2. β-Model [2]. We used the values of the parameter β obtained in experiments on dissociation of diatomic molecules in strong shock waves.

3. Coupled vibration-dissociation model (CVDV model) [9]. The dissociation rate depends significantly on the parameter $U = D/q$ (the value of q varies within the range $q = 3$–8). In the case of equiprobable dissociation from all vibrational levels, we have $U = \infty$, which corresponds to Hammerling's model [10]. With decreasing U, the probability of dissociation increases with increasing level number.

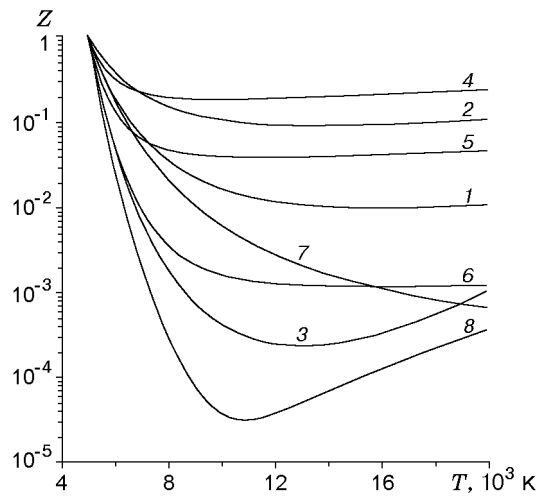

Fig. 1

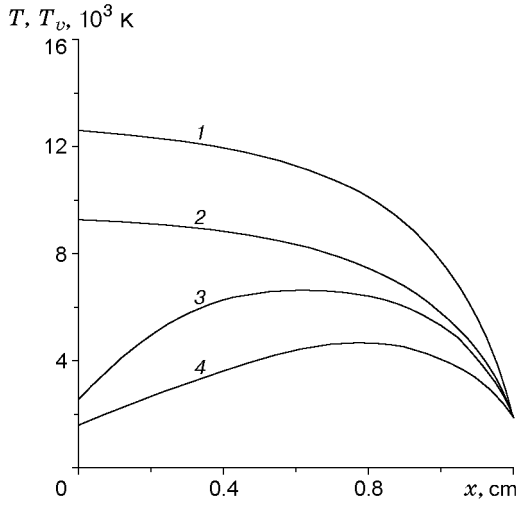

Fig. 2

4. Model of dissociation of the anharmonic oscillator (Kuznetsov's model [3]). The model is based on the assumption that molecular dissociation starts from the upper vibrational levels. The effective vibrational level $v = n^*$ divides the regions of fast and slow VV exchange by vibrational quanta, as compared to vibrational–translational transitions, in the space of vibrational energy.

5. Macheret and Fridmann's model [11]. The model is based on the use of general theoretical concepts of the kinetics of dissociation of vibrationally excited molecules with allowance for the solution of the dynamic problem of collision of a dissociating molecule with an atom or another diatomic homonucleous molecule. The model reveals the important role of translational energy of colliding particles in the process of dissociation of diatomic molecules at a high gas temperature.

Figure 1 shows the variation of the nonequilibrium parameter $Z(T, T_v) = k_d(T, T_v)/k_d^0(T)$ [2] [$k_d(T, T_v)$ and $k_d^0(T)$ are the nonequilibrium (two-temperature) and equilibrium rate constants of molecular dissociation, which were obtained by using different models of dissociation of the N_2 molecule]: curves 1 and 2 refer to Park's model [1] for $s = 0.5$ and 0.7, respectively, curve 3 refers to β-model [2], curves 4, 5, and 6 refer to CVDV model [9] for $U = \infty$, $D/3$, and $D/8$, respectively, curve 7 refers to Kuznetsov's model [3], and curve 8 refers to Macheret and Fridmann's model [11]. The vibrational temperature was assumed to be 5000 K, and the translational temperature varied from 5000 K to 20,000 K. The difference in nonequilibrium parameters determined by various VDI models reaches four orders for $T = 10{,}000$ K, which leads to a significant difference in concentrations of atoms and molecules in simulation of nonequilibrium flows. It follows from Fig. 1 that the dependence $Z(T, T_v)$ has a minimum with increasing gas temperature (for $T_v < T$) in some models. If the translational temperature is only slightly higher than the vibrational temperature, the main role in dissociation in these models belongs to transitions from the upper vibrational levels. With increasing gas temperature, the values of $Z(T, T_v)$ decrease because of the relative decrease in population of vibrationally excited states from which dissociation is possible. If the translational temperature of the gas becomes high, the role of direct dissociation of unexcited molecules increases, and the values of $Z(T, T_v)$ become higher. The position of the minimum of $Z(T, T_v)$ corresponds to the transition to dissociation from lower layers predominantly.

Figure 2 shows the calculation results obtained using the full Navier–Stokes equations and the kinetic scheme including the CVDV model ($U = D/3$) [9], namely, the distributions of translational temperature T (curve 1) and vibrational temperatures of NO, O_2, and N_2 molecules (curves 2, 3, and 4, respectively) along the critical streamline in an air flow around a body with a spherical bluntness of radius $R = 10$ cm (the coordinate $x = 0$ corresponds to the shock-wave position located at a distance of 1.2 cm from the body). The flight velocity $V_\infty = 5.1$ km/sec and altitude $H = 71$ km correspond to one point on the trajectory of the "Bow Shock-2" spacecraft. Figure 2 demonstrates significant vibrational nonequilibrium of nitrogen, oxygen, and nitric oxide molecules in the shock layer. This circumstance allows us to conclude that VDI has a strong effect on ionization and radiation characteristics of the flow in the shock layer, which is confirmed by the calculated data on the intensity of nonequilibrium radiation I integrated across the shock layer along the critical streamline, which are plotted in Fig. 3. The calculations are

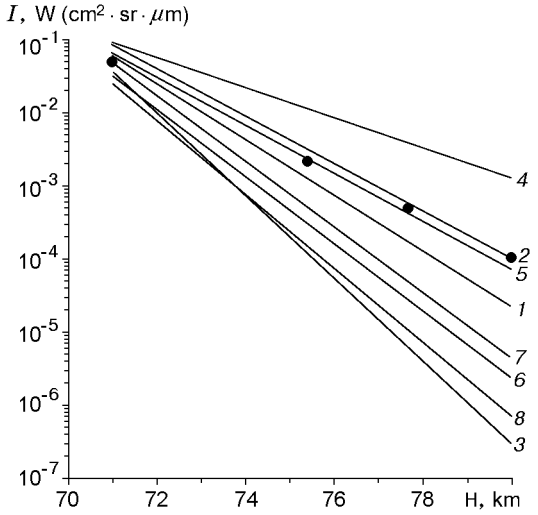

Fig. 3

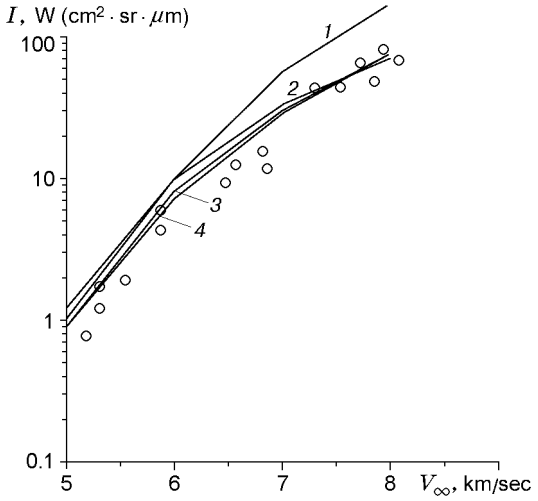

Fig. 4

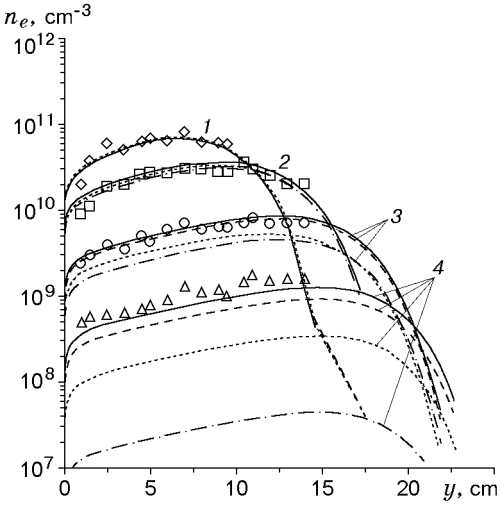

Fig. 5

performed for the flight conditions of the "Bow Shock-2" spacecraft (constant flight velocity $V_\infty = 5.1$ km/sec and $H = 71$–80 km) with the use of different VDI models: curves 1 and 2 refer to Park's model [1] for $s = 0.5$ and 0.7, respectively, curve 3 refers to β-model [2], curve 4 refers to model of equilibrium dissociation, and curves 5 and 6 refer to CVDV model [9] for $U = D/3$ and $D/8$, respectively, curve 7 refers to Kuznetsov's model [3], and curve 8 refers Macheret and Fridmann's model [11]. The points show the experimental results of [6].

The best agreement with the in-flight experiment is obtained by using Park's model of vibration–dissociation interaction [1] for $s = 0.7$ and the CVDV model [9] for $U = D/3$. The radiation intensities in the band system of NO(γ), which were obtained, for instance, with the use of Macheret and Fridmann's model [11], differ from the experimental values by more than two orders of magnitude at an altitude $H = 80$ km. With decreasing flight altitude, the influence of the choice of the VDI model on radiative characteristics of the shock layer decreases, and most VDI models under study yield close values of radiation intensity.

Similar results were obtained in numerical simulation of the flow behind strong shock waves, which was conducted by Gorelov et al. [4] who studied the channels of formation of nonequilibrium radiation of NO(γ) in the relaxation region, using the measurement results obtained in the electric-discharge shock tube of Central Aerohydrodynamic Institute. Figure 4 shows the maximum intensity of radiation in the spectral range $\lambda = (235 \pm 7)$ nm versus the shock-wave velocity. The pressure ahead of the shock-wave front is $P_1 = 13.3322$ Pa. The points are the experimental data; curve 1 refers to Park's model [1] for $s = 0.5$, curves 2 and 3 refer to the CVDV model [9] for $U = D/3$ and $D/8$, respectively, and curve 4 refers to Kuznetsov's model [3].

Figure 5 shows the numerical results for electron concentrations n_e, which were obtained for different VDI models, and also the measurement results obtained in flight conditions of the RAM-CIII vehicle [7]. The RAM-CIII vehicle was a blunted cone with a cone half-angle $\varphi = 9^\circ$ and spherical bluntness radius $R = 10$ cm. The flight velocity was $V_\infty = 7.65$ km/sec. The measurements were performed for $H = 71$, 76, 80, and 83.5 km at the trailing edge of the vehicle at a distance counted along the x axis from the critical point and equal to 1.3 m. The results in Fig. 5 confirm the previously made conclusions that the influence of the choice of the VDI model on ionization and radiation parameters becomes more substantial with increasing flight altitude. At an altitude $H = 71$ km, all the models used (the dashed curves refer to the CVDV model [9] for $U = D/3$, the solid curves to the β-model [2], the dot-and-dashed curves to the CVDV model [9] for $U = D/8$, and the dotted curves to Park's model [1]) yield the values of n_e that almost coincide with each other and with the measurement results (points and curves 1). With increasing flight altitude, the numerical data start to deviate from the measurement results [points and curves for $H = 76$ (2), 80 (3), and 83.5 km (4)]. Good agreement with flight results for all values of H is ensured only by numerical results obtained with the use of VDI models in [2, 9].

Generalizing the results of verification of the VDI model in terms of ionization parameters and similar verification in terms of radiative characteristics, we should note that the best agreement is obtained between the numerical data obtained using the VDI model [9] and the in-flight experiments [6, 7].

Conclusions. In numerical simulation of a nonequilibrium flow in the shock layer near a vehicle flying in air, the choice of the model of vibration-dissociation interaction has a strong effect on the kinetic processes and, hence, on ionization and radiation parameters of the flow. This effect is most significant for the vehicles examined in the present work ($R \approx 10$ cm and $V_\infty = 5$–8 km/sec) for $H > 75$ km.

The author is grateful to V. A. Gorelov, M. K. Gladyshev (deceased), and A. Yu. Kireev for their assistance in this work and to S. A. Losev and G. D. Smekhov for fruitful discussions.

This work was supported by the Russian Foundation for Fundamental Research (Grant No. 01-01-00467).

REFERENCES

1. C. Park, *Nonequilibrium Hypersonic Aerodynamics*, John Wiley and Sons, New York (1990).
2. G. G. Chernyi and S. A. Losev (ed.), *Physicochemical Processes in Gas Dynamics: Handbook* [in Russian], Izd. Mosk. Univ., Moscow (1995).
3. N. M. Kuznetsov, *Kinetics of Monomolecular Reactions* [in Russian], Nauka, Moscow (1982).
4. V. A. Gorelov, M. K. Gladyshev, A. Yu. Kireev, et al., "Experimental and numerical study of nonequilibrium ultraviolet NO and N_2^+ emission in shock layer," *J. Thermophys. Heat Transfer*, **12**, No. 2, 172–180 (1998).
5. V. A. Gorelov, M. K. Gladyshev, A. Yu. Kireev, et al., "Nonequilibrium ionization and radiation behind shock wave in the Martian atmosphere," in: *Proc. of the 3rd Europ. Symp. on Aerothermodynamics for Space Vehicles*, ESA Publ., Noordwijk (1998), pp. 429–436.
6. D. A. Levin, G. V. Candler, R. L. Collins, et al., "Examination of ultraviolet radiation theory for bow shock rocket experiments," AIAA Paper No. 92-2871 (1992).
7. J. S. Evans, C. J. Schexnayder, and P. W. Huber, "Boundary layer electron profiles for high-altitude entry of a blunt slender body," *AIAA J.*, **11**, No. 10, 1371–1372 (1973).
8. L. A. Kuznetsova and S. T. Surzhikov, "Atlas of spectral sections of absorption of electron and vibrational band systems of diatomic molecules," Preprint No. 603, Institute of Problems of Mechanics, Moscow (1997).
9. C. E. Treanor and P. V. Marrone, "Effect of dissociation on the rate of vibrational relaxation," *Phys. Fluids*, **5**, No. 9, 1022–1026 (1962).
10. P. Hammerling, J. Teare, and B. Kivel, "The radiation from luminous shock waves in nitrogen," *Phys. Fluids*, **2**, No. 10, 356–359 (1959).
11. S. O. Macheret, A. A. Fridmann, I. V. Adamovich, et al., "Mechanism of nonequilibrium dissociation of diatomic molecules," AIAA Paper No. 94-1984 (1994).