Monte Carlo Simulation of Re-Entry Flows Using a Bimodal Vibration Model

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The role of vibration-dissociation coupling in flows representative of aeroassisted transfer vehicles with afterbodies is considered. The physical model employed is motivated by the recent work of Sharma et al.[4] In this model, a bimodal representation, determined by the vibrational levels, is assumed for each diatomic molecule. Only molecules in the upper states are allowed to dissociate. The model is incorporated into the direct simulation Monte Carlo method of Bird and used to calculate steady flows past two geometries: a 5-deg blunt wedge and the project Fire configuration. Five chemical species are considered. It is shown that the new model results in reduced dissociation. Moreover, the convective heating rate increases for a finite catalytic wall and is essentially the same for a fully catalytic wall. Finally, for the conditions studied, the effect of the afterbody on the pressure distribution, heat transfer, and skin friction is minimal.

Introduction

CURRENT designs of aeroassisted transfer vehicles (AOTV) are characterized by an aeroshell with a large frontal area followed by an afterbody consisting of the payload. The thicker shock layer resulting from a very blunt aeroshell has the tendency of lowering the convective heating and increasing the radiative heating. Estimates of heat loads are usually determined from calculations based on the frontal area. One of the objectives of this work is to estimate the manner in which the afterbody affects the heat load.

The calculation of a complete configuration dictates the simultaneous consideration of two distinct phenomena. These phenomena are a result of the flow experiencing a compression in the shock layer followed by a rapid expansion around the afterbody. The mechanisms of vibrational relaxation and chemical reactions in an expanding gas are quite different from those of a gas going through a compression. The shock wave flow involves an approach toward an equilibrium state, whereas an expanding flow is characterized by a departure from equilibrium toward a frozen nonequilibrium state. Furthermore, the nonequilibrium processes in compression generally absorb energy and thus promote excitation in the shock layer, but in an expanding flow the processes release energy resulting in dexcitation.

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Diatomic molecules behave like anharmonic oscillators with vibrational energy gaps monotonically decreasing with the vibrational quantum numbers. Vibrational energy transfer in the diatomic gases are a result of vibration-vibration (V-V) exchange collisions and translation-vibration (T-V) exchange collisions.[1] The relative importance of these mechanisms depend on the temperature and vibrational level. At low temperatures, the V-V transitional probabilities are much larger than the T-V probabilities for the lower and intermediate vibrational levels and comparable for the higher levels. Thus, the energy mismatch resulting from anharmonicity and the disparity in the excitation rates hamper the energy transfer between the high and low vibrational levels. As a result, a bottleneck is created. This takes place whether one deals with an expansion[2] or a compression.[3]

In a recent paper, Sharma et al.[4] used an extension of the Schwartz, Slawsky, and Herzfeld (SSH) approximation to study coupled vibration dissociation in nitrogen. They showed that the fastest transitions are among the higher vibrational states and between these states and the free states. Thus, molecules in the higher vibrational states dissociate readily. As a result, the higher and lower vibrational states reach separate quasiequilibrium distributions. The findings reaffirm the existence of a bottleneck and serve as a basis for modeling the coupled vibration-dissociation process.

A biomodal representation is assumed for each diatomic molecule with the subdivision being based on the vibrational state of the molecule. As a result, dissociation is treated as a two-step process. Only molecules in the upper states are allowed to dissociate. This model is incorporated into the direct simulation Monte Carlo (DSMC) method of Bird.[5] Traditionally, the DSMC is implemented using a vibrational relaxation collision number independent of temperature and species. For an AOTV, the temperature of the flow changes drastically as it expands around the body. Therefore, it is necessary to incorporate in the method a vibrational relaxation collision number which is both temperature and species dependent. This number was derived from the data of Millikan and White[6] and an empirical adjustment suggested by Park.[7]

One would expect that the vibrational relaxation collision numbers for the various subspecies to be different. In the

absence of any data, these numbers were adjusted in an empirical manner.

Despite the fact that ionization and radiation may be important for the project Fire configuration, all calculations presented have used the five chemical species N_2, O_2, NO, N, and O. This was motivated by the desire to concentrate on the vibration-dissociation coupling phenomenon.

Formulation of the Problem

The DSMC method of Bird provides a general physical frame work for the study of complex flowfields.[8] However, because it is a direct simulation method, any results from a flow calculation are dependent on the physical model employed for that calculation. The approach used in this work takes advantage of the modifications to the DSMC procedure discussed in Ref. 9. The code used in Ref. 9 employs a constant value for the vibrational relaxation collision number irrespective of temperatures and species.

Early estimates of the vibrational relaxation rate relied heavily on Millikan and White's correlation of available experimental data. The correlation made use of the Landau-Teller theory of vibrational relaxation which has a limited range of applicability. As a result, Millikan and White's correlations are not valid at high temperatures. To remedy the situation, Park[7] suggested an empirical correlation. As a result of this correction, the vibrational relaxation time τ is given by

$$\tau = \tau_L + \tau_{cs} \tag{1}$$

where[6]

$$\tau_L = \frac{1}{p}\exp[A(T^{-1/3} - 0.015\mu^{1/4}) - 18.42]$$

$$A = 1.16 \times 10^{-3}\mu^{1/2}\Theta_v^{4/3} \tag{2}$$

and[7]

$$\tau_{cs} = \frac{1}{c_s \sigma_v n_s}$$

$$c = \sqrt{\left(\frac{8kT}{\pi m}\right)}, \qquad \sigma_v = 10^{-21}(50{,}000/T)^2, m^2 \tag{3}$$

In the above equation, p is the pressure in atmospheres, T the translational temperature in degrees Kelvin, Θ_v the characteristic vibrational temperature, μ the reduced mass, k the Boltzmann constant, and m_s and n_s give the particle mass and number density of species s, respectively.

To obtain the vibrational relaxation collision number, the quantity τ must be multiplied by the collision frequency v. The average collision frequency v_s for species s is given by

$$v_s = \sum (n_q \sigma_{T_{sq}} c_{r_{sq}}) \tag{4}$$

where $\sigma_{T_{sq}}$ is the total collision cross section for collisions involving particles s and q. This cross section is calculated using the relative velocity of particles s and q.

The quantity

$$\frac{1}{R} \equiv \frac{1}{\tau v} \tag{5}$$

determines the probability of a vibrational relaxation for a given collision. Thus rather than use a fixed value for all temperatures and species, the preceding expression helps bridge the gap between the physical models used in the current implementation of the DSMC and the Navier-Stokes calculations.[11]

The DSMC procedure calculates energies and not temperatures. Thus, the conceptually difficult problem of determining an appropriate temperature for a nonequilibrium flow does not have to be addressed. However, using the expressions for the equilibrium translational or internal energies, estimates of the translational, rotational, or vibrational temperature can be obtained at any stage in the flow calculation. This estimate of the temperature may be used to determine the bimodal representation.

The vibrational energy e_v for a diatomic molecule is given by

$$e_v = \frac{k\Theta_v}{\exp(\Theta_v/T) - 1} \tag{6}$$

The expression for e_v can also be written as

$$e_v = 0.5\zeta_v kT \tag{7}$$

where ζ_v is the number of excited vibrational degrees of freedom. For a given e_v, Eq. (6) is used to calculate the corresponding T and Eq. (7) is used to calculate ζ_v. Because ζ_v can range from zero to two, corresponding to temperatures ranging from zero to infinity, the value of ζ_v is used to assign each diatomic molecule to the appropriate mode. Thus, molecules with $\zeta_v < 1$ are assigned to the lower mode, and the remaining molecules are assigned to the upper mode.

As indicated, only diatomic molecules with $\zeta_v > 1$ are allowed to dissociate. The probability for a successful reaction is determined from a reaction cross section that will yield the experimentally measured rate coefficient for the reaction under consideration. It should be emphasized that the reaction cross section is independent of the temperature that appears in the experimentally measured rate coefficient. This is a significant observation because results of continuum calculations using a two-temperature model are dependent on the form of the model.

The results of Ref. 4 show that the vibrational relaxation rates for the lower and higher vibrational levels are quite different. In the absence of reliable data, the vibrational relaxation rates for the two modes are related by a constant multiplier. If rates become available, they can be easily incorporated into the calculation.

Results and Discussion

Two geometries were considered for this investigation. The first is the cylindrically blunted 5-deg half-angle wedge with a nose radius of 0.0254 m and length of 0.2 m. The freestream velocity was 7.5 km/s at an altitude of 80 km. The second is the project Fire configuration shown in Fig. 1. The freestream velocity was 11.35 km/s at an altitude of 84.7 km. In both calculations, surface temperature is 1000 K and the catalytic recombination coefficient is 0.003 when a finite catalytic condition is assumed.

One of the objectives of this work is to study the role of vibration-dissociation coupling in nonequilibrium hypersonic flows in the presence of compression and expansion. The other objective is to assess the influence of the afterbody on heat

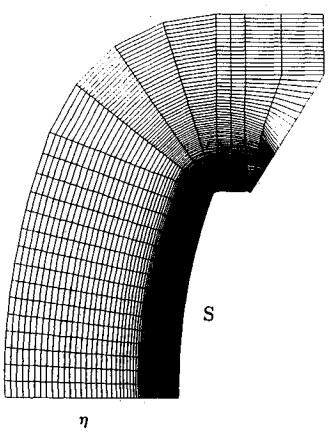

Fig. 1 Grid for project Fire vehicle.

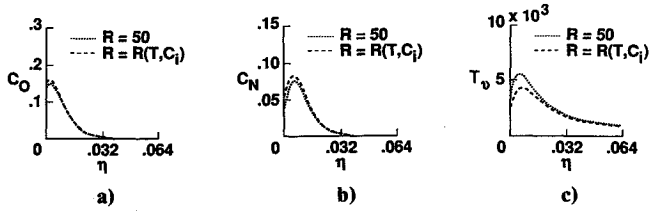

Fig. 2 Effects of variable relaxation number on properties along stagnation streamline (5-deg wedge): a) concentration of oxygen atoms; b) concentration of nitrogen atoms; and c) vibrational temperature.

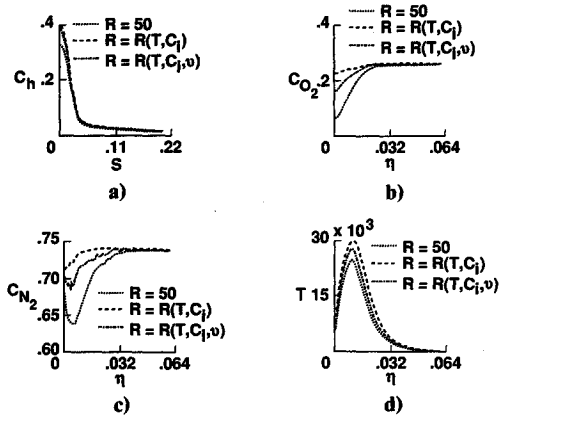

Fig. 3 Effects of bimodal concept (5-deg wedge): a) concentration of oxygen atoms; b) oxygen concentration; c) nitrogen concentration, and d) translational temperature.

transfer and pressure distribution. Because of this, all calculations were carried out for the five chemical species N_2, O_2, NO, N, and O. Most of the calculations were carried out for a finite catalytic wall condition.

All of the proposed changes were first tested and compared with the traditional DSMC using the 5-deg wedge. This was done for two reasons: simpler geometry and lower freestream velocity. The first change examines the effect of using a temperature- and species-dependent vibrational relaxation number R. The results show that the change has an insignificant influence on coefficients of heat transfer C_h, pressure C_p, and skin friction C_f. The observable effects are shown in Fig. 2 where the distributions of the concentrations of N and O, C_N and C_O, and the vibrational temperature T_v along the stagnation streamline are indicated. This result is somewhat remarkable because the vibrational relaxation number used in the traditional DSMC is 50 while the temperature and species dependent number, which is always greater than 50, varied by three orders of magnitude.

The next calculation shows the influence of the biomodal concept. As is seen from Fig. 1 of Ref. 4, the vibrational transitional rate coefficient for the higher vibrational levels is much higher than the corresponding rate for the low vibrational levels. Thus, to assess the influence of the concept, two calculations were carried out and compared with the traditional DSMC. The first assumes that $R = R(T,C_i)$ independent of the vibrational levels v, where C_i is the concentration of species i, while the second assumes a reduction in R by a factor of 25 for the higher vibrational levels, and thus $R = R(T,C_i,v)$. This results in a decrease of the vibration relaxation number for the higher levels. Figure 3 clearly illustrates that the bimodal concept results in a reduction of dissociation and an increase in the translational temperature and heat transfer. The reduction in dissociation is a result of the fact that only a fraction of the molecules are in the upper vibrational levels where dissociation is permitted. With reduced dissociation, less energy is being consumed in breaking up the molecules and more energy remains in the translational mode. Thus, the convective heating is increased. On the other hand, reducing the vibrational relaxation number for the higher vibrational modes increases the excitation rates. This results in an increase in the vibrational temperature and the amount of dissociation and, in turn, a reduction in the translational temperature and heat transfer.

Two-temperature models were introduced by Park[7] to account for the fact that a one-temperature description of reaction rates leads to a substantial overestimation of the rate of dissociation. By considering reaction rates that depend on both the translational and the (lower) vibrational temperature, he obtains reduced rates of dissociation and a better agreement of theory with experiment. However, since the exact functional dependence of the rates on vibrational temperature is unknown at present, his formulations are of a semiempirical nature. The results of Fig. 3 and subsequent results show that a reduction in the dissociation rates is possible without having to rely on semiempirical two-temperature models.

The next series of calculations to be examined are for the project Fire configuration. One of the difficulties of including afterbodies in DSMC calculations is that a lengthy calculation is needed to accumulate a meaningful sample in the afterbody region. Figure 4 compares calculations obtained for the complete body and for the front portion only using the traditional DSMC. As is seen from the figure, the presence of the afterbody has little influence on the heat transfer, pressure distribution, and skin friction. This suggests that the flowfield in the region of the afterbody can be calculated, with minor error, by using initial conditions obtained from the frontal portion only. Such a procedure would result in reduced computation time.

Figure 5 shows the influence of the bimodal concept for the whole project Fire configuration where $R = R(T,C_i)$ is independent of the vibrational levels. Again, the reduced dissociation results in an increase in the convective heat transfer. The increase in the convective heating is more pronounced than for the wedge because of the increase in the freestream velocity and the bluntness. Figure 6 compares, for the forebody of the project Fire configuration, the traditional DSMC calculation with two calculations employing the bimodal concept. These two calculations assume, respectively, that $R = R(T,C_i)$ and $R = R(T,C_i,v)$. The results confirm earlier observations that use of a bimodal concept increases the convective heating. Moreover, using a lower vibrational number for the higher vibrational states reduces the convective heating.

All of the preceding results assumed a finite catalytic surface. The next set of calculations assume a fully catalytic sur-

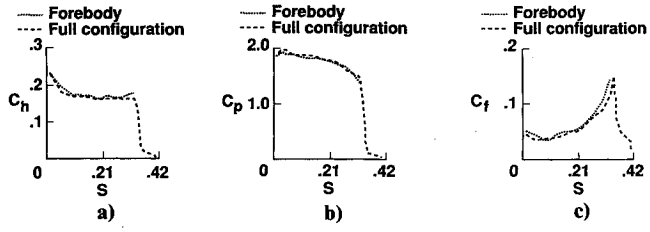

Fig. 4 Effect of afterbody on surface properties (project Fire): a) heat-transfer coefficient; b) pressure coefficient; and c) skin-friction coefficient.

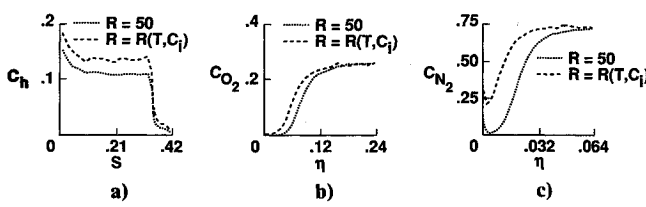

Fig. 5 Effects of bimodal concept (project Fire, complete configuration): a) heat-transfer coefficient; b) oxygen concentration; and c) nitrogen concentration.

face. Only results for the 5-deg wedge are presented. Figure 7 shows that although the bimodal assumption results in reduced dissociation, the convective heating remains the same. This is because all energy expended in dissociation is recovered at the surface as a result of atom recombination. The calculation also assumes $R = R(T,C_i,\upsilon)$, which results in increased vibrational relaxation for the high vibrational levels and thus an increase in vibrational temperature.

The role of nonequilibrium vibrational relaxation and the use of a two-temperature model have been investigated by Brown.[12] He showed that the heat transfer is increased by vibrational relaxation when a noncatalytic wall condition is employed but remains the same when a fully catalytic wall assumption is made. This conclusion is in agreement with the present findings.

The preceding calculations are carried out to illustrate the impact of a bimodal vibration model on re-entry flows. Because ionization and radiation were not considered, no attempt was made to compare the Fire II data.[13] Even though the Fire II configuration was considered at a velocity and altitude that corresponds to 1631 s into the mission, the surface conditions used, i.e., 1000 K and a catalytic recombination coefficient of 0.003, were more representative of the Shuttle surface. If it is assumed that ionization and radiation are negligible at the 1631-s point in the mission, then the preceding calculations can be used to evaluate the bimodal vibration model. The surface temperature at that time was in the range 450-475 K. Because the surface was exposed to the atmosphere, beryllium oxide (BeO) was formed. The value of the catalytic recombination coefficient for such a surface at the indicated temperature is about 0.02.[4] The measured C_h at S/R of 0.09 corresponds (by pure accident) to the value corresponding to $R = 50$ in Fig. 5. If it is recalled that such a calculation was made for a $Tw = 1000$ K and a catalytic recombination coefficient of 0.003, any calculation for a lower surface temperature and a higher catalytic recombination coefficient will be higher than the measured value. Thus, even when the bimodal vibration model is not employed, DSMC will overpredict C_h. Since the bimodal model overpredicts the convective heating, one would be inclined to conclude that such a model is inappropriate. On the other hand, when ionization is taken into consideration, C_h will be reduced. Thus, in order to settle the issue, allowance for ionization must be made.

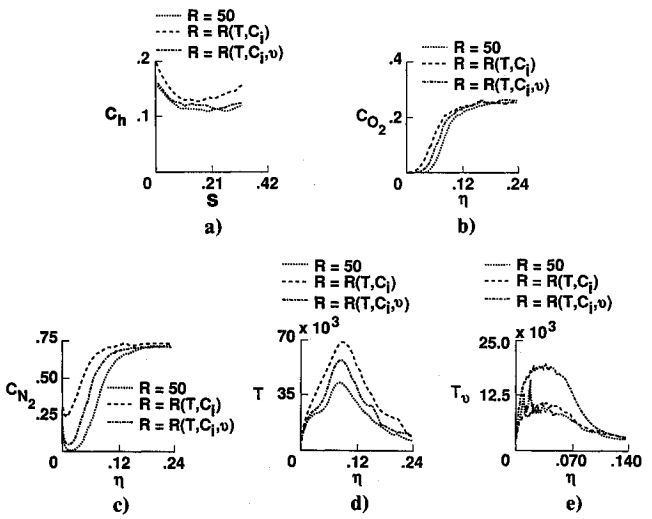

Fig. 6 Effects of bimodal concept (project Fire, forebody only): a) heat-transfer coefficient; b) oxygen concentration; c) nitrogen concentration; d) translational temperture; and, e) vibrational temperture.

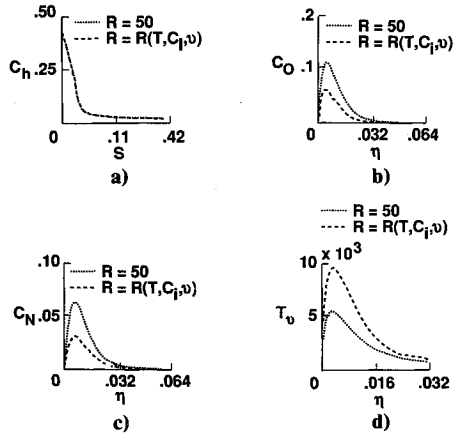

Fig. 7 Effect of fully catalytic wall (5-deg wedge): a) heat-transfer coefficient; b) atomic oxygen concentration; c) atomic nitrogen concentration; and d) vibrational temperature.

Let us consider next the continuum calculations. Gnoffo[15] took ionization into consideration and assumed a fully catalytic surface. His results are in excellent agreement with experiment. Had he assumed a more representative value of the catalytic recombination coefficient, his predictions would have been lower than experiment. The use of a two-step dissociation model, i.e.,

$$N_2 + M \rightarrow N_2^* + M$$

$$N_2^* + M \rightarrow N + N + M$$

which is equivalent to the procedure implemented in DSMC, will result in reduced dissociation and increased heating. Thus, in this case one is inclined to conclude that such a model would be appropriate.

It is evident from the preceding discussion that additional computations and comparisons with experiment are needed to settle the issues raised by the bimodal vibration model.

Concluding Remarks

A physical model designed to reflect the correct behavior of anharmonic diatomic molecules at high temperatures has been developed and incorporated into the DSMC of Bird. The model results in reduced dissociation and increased convective heating for flows with finite catalytic surfaces.

When dealing with flowfields where both compression and expansion takes place, it is important to use temperature- and species-dependent vibrational relaxation numbers. This is because of the wide variation in the values of these numbers with temperature.

Finally, it appears that the effects of the afterbody on flows typical of an AOTV are minimal in the absence of ionization and radiation. This makes it possible to calculate the flow about a full configuration by first calculating the forebody and then using the results to calculate the afterbody.

Acknowledgments

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