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Direct Simulation with Vibration-Dissociation Coupling

David B. Hash* and H. A. Hassan†
North Carolina State University, Raleigh, North Carolina 27695

In the investigation of hypersonic rarefied flows, it is important to consider the effects of thermal nonequilibrium on the dissociation rates. Because the vibrational mode requires a finite time to relax, vibrational energy may not be available for dissociation immediately behind the shock. In this way, the dissociation of the preshock species can be delayed for a significant portion of the hypersonic shock layer. The majority of implementations of the direct simulation Monte Carlo (DSMC) method of Bird do not account for vibration-dissociation coupling. Haas and Boyd have proposed the vibrationally favored dissociation (VFD) model to accomplish this task. Their model made use of measurements of induction distance to determine model constants. A more general expression has been derived that does not require any experimental input. The model is used to calculate one-dimensional shock waves in nitrogen and the flow past a lunar transfer vehicle (LTV). For the conditions considered in the simulation, the influence of vibration-dissociation coupling on heat transfer in the stagnation region of the LTV can be important.

Nomenclature

c_m = mean thermal speed
c_r = relative velocity
D = dissociation energy
E_a = activation energy
E_c = collision energy
E_v = vibrational energy of dissociating molecule
f = distribution function
g = Hinshelwood distribution
k = Boltzmann constant
k_f = reaction rate coefficient
l = characteristic dimension
m = particle mass
n = number density
P = pressure
Pr = steric factor
P_{relax} = relaxation probability
R_n = nose radius
S = surface coordinate
T = temperature
T_t = translational temperature
T_v = vibrational temperature
u_∞ = upstream velocity
Y_N = mass fraction of atomic nitrogen
Z = relaxation number
α = temperature exponent for Arrhenius expression
β = beta function
Γ = gamma function
δ = symmetry factor
$\overline{\varepsilon_v}$ = average vibrational energy removed during dissociation
ζ = internal degrees of freedom (DOF)
ζ_v = vibrational DOF of dissociating molecule
η = inverse power law exponent
θ_v = characteristic vibrational temperature
λ_∞ = freestream mean free path
μ = reduced mass
ν = collision frequency
ξ = radial coordinate
σ_T = total collision cross section
τ = relaxation time
ϕ = VFD exponent
Ω = degree of vibrational nonequilibrium
ω = VHS exponent

Introduction

THE shock layer on an aerobrake during its high altitude pass will exhibit a significant region of thermal and chemical nonequilibrium. During the thermal nonequilibrium portion of the flow, the particles evolve from their preshock ground state to a vibrationally excited nonequilibrium state. Since vibrationally excited particles are much more likely to dissociate, the dissociation process is delayed in the thermal nonequilibrium region.

Much work has concentrated on determining the degree to which vibrational nonequilibrium delays dissociation. The coupled-vibration-dissociation-vibration (CVDV) model of Marrone and Treanor[1] attempts to account for the preferential removal of vibrational energy by dissociation with the Landau-Teller model of the simple harmonic oscillator. The CVDV model showed that $\overline{\varepsilon_v}$ is

$$\tfrac{1}{2} \leq (\overline{\varepsilon_v}/D) \leq 1 \tag{1}$$

A more recent investigation by Landrum and Candler[2] using an anharmonic oscillator with a vibrational energy transfer model developed by Schwartz et al.[3] (SSH theory) and modified by Keck and Carrier[4] showed that

$$(\overline{\varepsilon_v}/D) \approx 1 \tag{2}$$

Thus, most of the energy used in dissociation is vibrational energy. These results show that the rate of dissociation is very dependent on the vibrational state of the gas and that vibrational nonequilibrium can significantly slow the dissociation process.

Most of the above theories ignore the effects of rotation-vibration coupling. This is consistent with assuming the total energy to be a linear sum of individual energies. If this is relaxed, then rotation-vibration coupling should be considered.

The DSMC method of Bird[5] has been very useful in the investigation of rarefied gas flows. However, most of the cur-

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*Research Assistant, Mechanical and Aerospace Engineering. Student Member AIAA.

†Professor, Mechanical and Aerospace Engineering. Associate Fellow AIAA.

rent implementations of the method do not account for vibration-dissociation coupling. This may produce inaccurate solutions for flows of significant thermal nonequilibrium. Haas and Boyd[6] have recently developed the vibrationally favored dissociation (VFD) model in order to account for the coupling. This is accomplished by choosing an expression for the dissociation probability that is a function of the vibrational energy

$$Pr \sim E_v^{\phi} \tag{3}$$

where ϕ is determined by matching simulated results to experimentally measured induction distances. They simulated several relaxation zones behind different shock waves of nitrogen flows and then compared them to induction distance measurements made by Hornung[7] to determine ϕ for nitrogen dissociation. Evidently, the relative size of the induction distance behind the bow shock measured in Ref. 7 is somewhat dependent on the radius of the cylinder employed. In addition, establishing the size of the induction distance in "which no appreciable dissociation occurs" is somewhat subjective. Finally, in situations where a number of dissociation reactions proceed simultaneously, it is not clear how a measurement of an induction distance can be used to determine the various model constants required. As a result, a new approach is developed that does not require any experimental input, i.e., it does not require any additional parameters beyond those appearing in the Arrhenius factor.

Before introducing the present model, a brief description of the DSMC technique is given. Secondly, the deficiencies of the conventional reaction model, i.e., where vibration-dissociation coupling is not considered, are described, and initial attempts by Haas and Boyd[6] to model vibration-dissociation coupling are discussed in more detail. Then, the derivation of a new form for the reaction probability is given. Next, density distributions are compared for one-dimensional nitrogen shock cases for the conventional model, the VFD model, and the present model. Finally, comparisons are made between the conventional model and the present model for the convective heat transfer rates on a lunar transfer vehicle (LTV) being considered by NASA-Marshall.

Physical Models in DSMC

Instead of analyzing a mathematical model of the flow, DSMC simulates the flow through the movement and collision of computational particles. The flowfield is represented by several thousand simulated particles, each representing a large number of real particles. The movement and collision of these particles are decoupled over a small time step, and the flowfield is partitioned into several thousand cells in which the collision process is executed.

Description of the collision process relies on three distinct models: 1) selection of an interaction potential and a collision probability; 2) the Larsen-Borgnakke Energy Partition method[8]; and 3) the chemical reaction model. In all three models, a probability of occurrence is determined and then compared to a random fraction between 0–1. The phenomenon occurs if the probability is larger than the random fraction. This is the so-called acceptance-rejection method. The following discusses the latter two models because of their importance in vibration-dissociation coupling. In order to properly account for the coupling, the probabilities for internal energy exchange and reaction used in the acceptance-rejection method must be accurately determined.

Internal Energy Exchange

The DSMC method attempts to accurately simulate energy relaxation rates, and thus the degree of thermal nonequilibrium, through the use of the Larsen-Borgnakke Energy Partition method to determine the postcollision partitioning of energy between the translational and internal modes. Of course, if both collision partners are monatomic, no partitioning occurs. In the case where either one or both particles are polyatomic, the collision energy must be partitioned. This method is implemented by assuming that a fraction of collisions are elastic. Of the fraction of collisions that are inelastic, all relax rotationally and a fraction of these relax vibrationally. These relaxation probabilities can be determined from measured relaxation times. The relaxation time is a function of the local flow properties and can be related to a relaxation number, the number of collisions it takes for a particular mode to attain equilibrium. Once this number is determined, the probability of relaxation for each mode in a given collision can be computed with the following expression:

$$P_{\text{relax}} = (1/Z) = (1/\nu\tau) \tag{4}$$

If the probability is greater than a random fraction, then the relaxation occurs in one collision whereby the postcollision energies are sampled from equilibrium distributions. This is nonphysical on a microscopic level since it takes many collisions for a mode to relax, but the method satisfies detailed balancing and gives correct macroscopic results for the relaxation rates.

As seen from the above, it is necessary to specify the relaxation numbers for the rotational and vibrational modes in order to compute the relaxation probabilities. Traditionally, DSMC uses a rotational relaxation number Z_R on the order of five. This means, on average, rotational relaxation occurs for one in every five collisions. A more realistic expression for the rotational relaxation number as a function of the translational temperature has been developed by Parker[9] where

$$Z_R = \frac{Z_{R,\infty}}{1 + (\pi^{3/2}/2)(T^*/T_t)^{1/2} + [(\pi^2/4) + \pi](T^*/T_t)} \tag{5}$$

with $Z_{R,\infty}$ being chosen as 16 and T^* as 91.5 K, suggested by Boyd[10] for nitrogen. The expression of Parker was implemented for the one-dimensional nitrogen shock calculations, but was excluded in the Lunar transfer vehicle (LTV) calculations because of lack of suitable constants, $Z_{R,\infty}$ and T^*, for oxygen and nitric oxide. For the LTV calculations, a constant rotational relaxation number of five was used for all diatomic species.

The vibrational relaxation number is also computed as a function of the flow properties. The relaxation number can be easily determined if the collision frequency and the relaxation time are known. Thus, in this work, the Millikan and White[11] expression is used to determine the vibrational relaxation time τ_v for any species and is given by

$$\tau_v = \tau_L + \tau_{cs} \tag{6}$$

where

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

$$A = 1.16 \times 10^{-3}\mu^{1/2}\Theta_v^{4/3} \tag{7}$$

$$\tau_{cs} = (1/c_{m,s}\sigma_\nu n_s)$$

$$c_{m,s} = \sqrt{(8kT/\pi m_s)}, \quad \sigma_v = 10^{-21}(50{,}000/T)^2, \quad m^2 \tag{8}$$

In the above equation, μ is the reduced mass of the collision partners; $c_{m,s}$, m_s, and n_s are the average thermal velocity, mass, and number density of species s, respectively; and Θ_v is the characteristic temperature of the vibrational mode of the diatomic species. τ_{cs} is a correction factor suggested by Park[12] as a limit, since the Millikan and White[11] formula gives unrealistically small relaxation times for high temperatures. In most cases, Park's correction is not needed because the vibrational relaxation number is not allowed to be less than the rotational relaxation number. Thus, the vibrational relaxation number, Z_V can be determined where

$$Z_V = \nu \tau_v \tag{9}$$

The above method accurately simulates the vibrational relaxation of the gas in the shock layer. However, the effect of vibrational nonequilibrium on the dissociation of the gas must be accounted for in the chemical reaction model.

Chemical Reaction Model

The purpose of this model is to accurately simulate reaction rates. This is accomplished through the determination of steric factors or probabilities of reaction. The steric factor is chosen so that, at equilibrium, it reproduces an Arrhenius form for the reaction rate coefficient where

$$k_f = AT^{\alpha} \exp(-E_a/kT) \tag{10}$$

From the definition of the reaction rate coefficient in the case of dissociation

$$k_f = \frac{\overline{\sigma_T c_r}}{\delta} \int_D^{\infty} Prf(E_c)\, \mathrm{d}(E_c) \tag{11}$$

with

$$f(E_c) = \frac{1}{\Gamma(\zeta - \omega + 2)kT} \left(\frac{E_c}{kT}\right)^{\zeta - \omega + 1} \exp\left(-\frac{E_c}{kT}\right)$$

$$\omega = \frac{2}{\eta - 1} \tag{12}$$

ζ is the average internal DOF that contribute to the reaction, and η is the exponent for the inverse power law interaction potential. δ is the symmetry factor which is 1 for unlike molecules and 2 for like molecules. For the variable-hard-sphere (VHS) model[13]

$$\overline{\sigma_T c_r} = \sigma_{\mathrm{ref}} \Gamma(2 - \omega) \left[(2 - \omega)\frac{T_{\mathrm{ref}}}{T}\right]^{\omega} \left(\frac{8kT}{\pi\mu}\right)^{1/2} \tag{13}$$

The function for the steric factor is not unique, in that kinetic theory does not provide an exact expression. Thus, a shape has to be assumed that meets certain physical constraints. First, it is required that the steric factor be zero at the threshold ($E_c = D$) and when the energy of collision is large ($E_c \to \infty$). Thus, Bird assumes the form of the steric factor to be the following:

$$Pr = \begin{cases} B(E_c - D)^m E_c^n, & E_c > D \\ 0, & \text{otherwise} \end{cases} \tag{14}$$

where B, m, and n are determined so that at equilibrium the expression for k_f matches Eq. (10). The value of m must be positive so that $Pr = 0$ at the threshold, and the sum of m and n must be negative so that Pr approaches zero as E_c becomes large. The resulting expression for the conventional model can be written as follows:

$$Pr = \frac{\delta\sqrt{\pi\mu/8A}}{\sigma_{\mathrm{ref}} k^{\alpha}[(2 - \omega)kT_{\mathrm{ref}}]^{\omega}} \frac{\Gamma(\zeta - \omega + 2)}{\Gamma(2 - \omega)\Gamma(\zeta + \alpha + \frac{3}{2})} \times (E_c - D)^{\zeta + \alpha + 1/2} E_c^{\omega - \zeta - 1} \tag{15}$$

If the energy of collision is greater than the activation energy, Pr is calculated. In the implementation of the acceptance-rejection method, the steric factor is compared to a random fraction varying between 0–1. If Pr is larger than the random fraction, then the reaction occurs.

As seen from the above, the steric factor is not explicitly dependent on the vibrational energy. However, the expression does not rule out a contribution of the vibrational modes to ζ.

Vibration-Dissociation Steric Factors

Recently, Haas and Boyd[6] examined vibration-dissociation coupling and developed the vibrationally favored dissociation (VFD) model. For the case of an anharmonic oscillator

$$\begin{gathered} k_f = \frac{\overline{\sigma_T c_r}}{\delta} \int_0^D \int_{E_a}^{\infty} Pr\, g(E_v)\, f(E)\, \mathrm{d}E\, \mathrm{d}E_v \\ E_a = D - E_v \\ E = E_c - E_v \end{gathered} \tag{16}$$

$g(E_v)$ is the Hinshelwood[14] distribution given by

$$g(E_v) = \frac{1}{\Gamma(\zeta_v/2)kT} \left(\frac{E_v}{kT}\right)^{(\zeta_v/2) - 1} \exp\left(-\frac{E_v}{kT}\right) \tag{17}$$

Haas and Boyd propose that the steric factor should have the following form:

$$Pr = \begin{cases} Q(E - E_a)^i E^j E_v^{\phi}, & E > E_a \\ 0, & \text{otherwise} \end{cases} \tag{18}$$

The additional term, E_v^{ϕ}, produces a steric factor which increases with vibrational energy. Therefore, the effects of vibrational nonequilibrium can be represented through ϕ. The exponent ϕ was treated as a free parameter to be determined from experimental measurements of induction distances. Obviously, theoretical treatments may be used to determine such parameters. It is not clear whether ϕ is reaction- and/or species-dependent, and it is not obvious how one would use the results of an experiment similar to that of Hornung for air or another gas mixture. In addition, the maximum of the function for a given E_v is

$$Pr_{\max} = Q\{-[i/(i + j)]^i [j/(i + j)]^j\}(D - E_v)^{i + j} E_v^{\phi} \tag{19}$$

Upon close examination, since the sum of i and j must be less than zero, the maxima of the steric factor is unbounded as E_v approaches D. This violates the requirement that Pr should be less than one.

Haas and Boyd[6] developed a different expression for the unbounded simple harmonic oscillator. The resulting expression is characterized by a $Pr_{\max}$ that remains bounded as $E_v \to D$. Because in a classical setting E_v cannot exceed D, the following considerations will be restricted to the bounded anharmonic oscillator.

The present investigation provides a more general steric factor expression which can be derived for VFD without having to appeal to experiment. Moreover, the approach can be employed for a gas mixture in the presence of any number of dissociation reactions. For this approach, the steric factor is chosen as

$$\begin{gathered} Pr = \begin{cases} Q(E - E_a)^i E^j (D - E_v)^{\psi} E_v^{\phi}, & E > E_a \\ 0, & \text{otherwise} \end{cases} \\ \psi = -(i + j) \end{gathered} \tag{20}$$

Using the above expression, it can be shown that for a given E_v

$$Pr_{\max} = Q\{-[i/(i + j)]^i [j/(i + j)]^j\} E_v^{\phi} \tag{21}$$

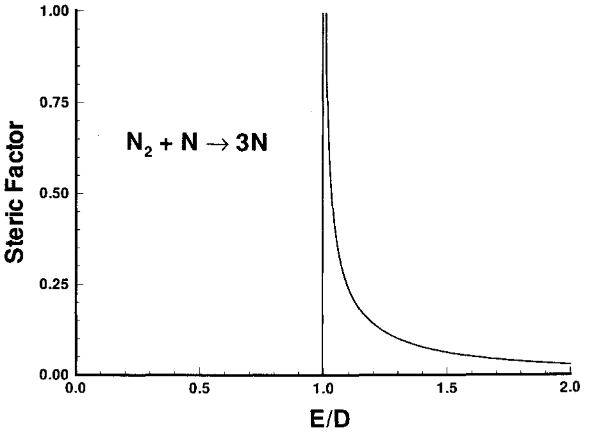

Fig. 1 Steric factor for dissociation of oxygen.

Since Pr is bounded by unity, ϕ is evaluated by that value that yields $Pr_{\max} = 1$ when $E_v = D$. The above procedure is adopted for each reaction resulting in dissociation. The remaining coefficients in Eq. (20) are determined in such a way as to reproduce the experimentally measured rates at equilibrium, and are given as

$$i = \zeta + \alpha + (\zeta_v/2) + \tfrac{1}{2}$$

$$j = \omega - \zeta - 1$$

$$\psi = \tfrac{1}{2} - \alpha - \omega - (\zeta_\nu/2)$$

$$Q = \frac{\delta\sqrt{\pi\mu/8}A}{\sigma_{\text{ref}}k^{\alpha}D^{\phi+(\zeta_v/2)+\psi}[(2-\omega)kT_{\text{ref}}]^{\omega}} \times \frac{\Gamma(1-j)\Gamma(\zeta_v/2)}{\Gamma(2-\omega)\Gamma(i+1)\beta[\psi+1, \phi+(\zeta_v/2)]} \tag{22}$$

With i, j, and Q determined, ϕ follows from Eq. (21) with E_v = D and $Pr_{\max}$ = 1.0.

Because the parameters in the Arrhenius rate expression are assumed given, there is no assurance that Eq. (21) will give a positive value for ϕ. Moreover, even if one accepts a zero value for ϕ, which will still yield an expression that favors dissociation from higher vibrational states, there is no assurance that $Pr_{\max}$ will be less than or equal to one. A case in point is the O_2 dissociation reaction of Park and Menes.[15] Figure 1 is a plot of the steric factor for the $O_2 + O \rightarrow 3O$ reaction with $\phi = 0$. As seen from the figure, $Pr_{\max}$ can exceed 1. In a situation like this, either an expression different from that given in Eq. (20) is necessary, or a different Arrhenius rate expression should be selected. Thus, use of the more recent rate of data of Park et al.[16] yield a value of ϕ which is positive and $Pr \leq 1$.

One-Dimensional Nitrogen Shock Calculations

In order to determine the VFD exponent, Haas and Boyd[6] computed several relaxation zones behind different shock waves and adjusted the value of ϕ until the calculations matched the experimental measurements of induction distances by Hornung. In this experiment, induction lengths were measured from interferograms of hypersonic flows of nitrogen around a blunt body. For the VFD anharmonic model, a value between 2–3 is suggested for ϕ for nitrogen flows. Haas and Boyd begin their calculations immediately behind the shock, assuming the translational and rotational modes are in equilibrium at the temperature calculated by Hornung[7] and that the vibrational temperature is 300 K. The present work simulates normal shock waves using upstream conditions given in Ref. 7 and assumes an upstream temperature of 300 K. The calculations are carried out for the conventional reaction model, the VFD model (ϕ = 2.5), and the present model. Haas and Boyd did not present any results using the Anharmonic VFD model. As a result, all calculations presented in this article have been carried out by the authors. The conditions for the cases considered are given in Table 1.

Dissociation reactions considered are:

$$\begin{aligned} &1.\ N_2 + N_2 \rightarrow N_2 + N + N \\ &2.\ N_2 + N \rightarrow N + N + N \end{aligned} \tag{23}$$

The rates of Appleton et al.[17] and Flagan and Appleton[18] are used for these calculations. Table 2 presents the rate constants and model exponents.

The only difference between the models is the expression for the steric factor. Figures 2–4 show the variation of the steric factor with vibrational energy for reaction 2. The steric factor that reproduces Appleton's rates at equilibrium, in the

Table 1 Case conditions

Case	u_∞, km/s	Y_N	$\rho_\infty \times 10^3$, kg/m^3	T_∞, K
1	5.6	0.07	5.0	300
2	8.8	0.65	1.8	300

Table 2 Reaction set for one-dimensional nitrogen shock calculations

Reaction	A	α	D/k	ϕ_{VFD}	ϕ
1	6.14×10^{-9}	−1.6	113,070	2.5	5.14
2	2.76×10^{-8}	−1.6	113,070	2.5	2.45

Units of A are m^3·particle^{-1}·s^{-1}.

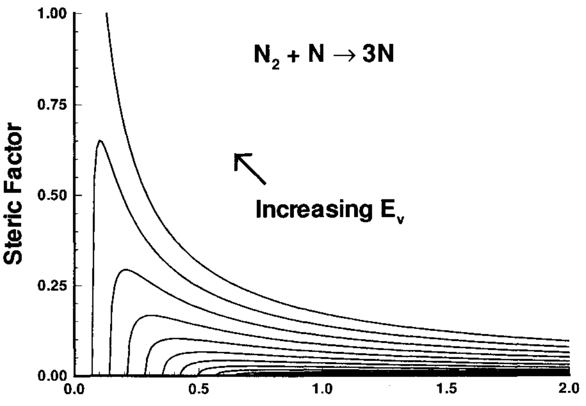

Fig. 2 Steric factor for conventional model (Appleton's rate).

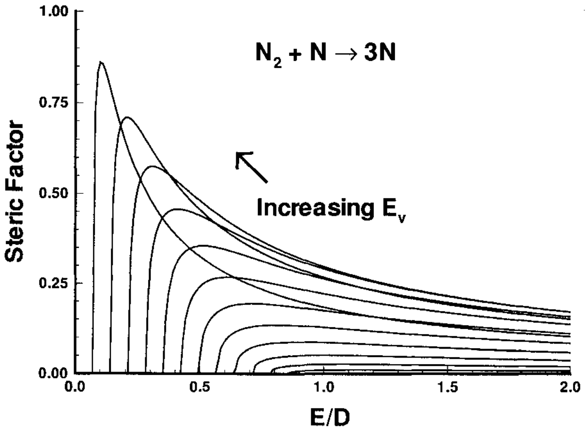

Fig. 3 Steric factor for VFD model.

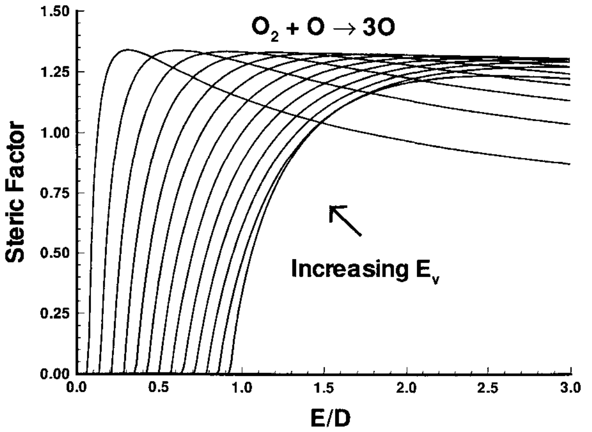

Fig. 4 Steric factor for new model.

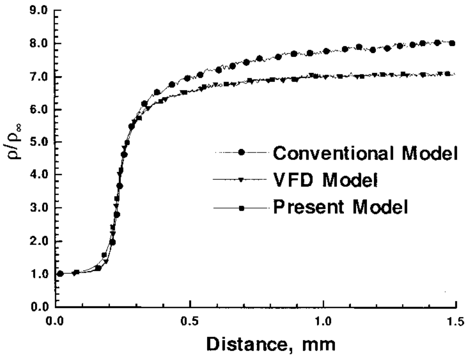

Fig. 5 Density distributions for case 1.

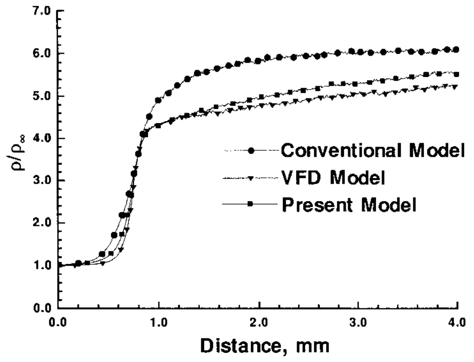

Fig. 6 Density distributions for case 2.

absence of vibration-dissociation coupling, is given in Fig. 2. For this reaction, ζ was chosen, assuming that only half of the rotational DOF contribute to the reaction. The resulting steric factor does not have the correct physical behavior at the threshold. This can easily be corrected by adjusting the value of α in Table 2 to a value slightly higher than -1.6, or by assuming a larger contribution from the rotational modes. Figure 3 shows that the anharmonic VFD model is unbounded when $E_v = D$. The present model corrects the problem with the VFD model and helps to diminish the problem with the conventional model without having to adjust the equilibrium rate parameters. The figures show the main feature of the vibration-dissociation steric factors; the maximum of the steric factor increases with vibrational energy. Thus, molecules in higher vibrational states have a higher probability for dissociation. Because it takes a finite time for a molecule in the ground state to be excited to a high vibrational level, a delay of dissociation will invariably result from using an expression similar to that given by Eq. (20).

Figures 5 and 6 give the density distributions for all the models for cases 1 and 2, respectively. Both the VFD model and the present model lag behind the conventional model. Since dissociation does not occur as quickly, the rate of change of the density is slower behind the shock for the vibrational nonequilibrium dissociation models. Moreover, the results for the present model compare very well to the VFD model.

Determining model constants by matching experimental measurements may not always be an option. For larger bodies, Hornung[19] did not observe an induction distance because of the scale of the experiment. Thus, if the induction distance depends on the scale of the experiment, then it is not a reliable procedure for determining model constants. The present model provides an easy way to incorporate vibration-dissociation coupling into DSMC.

Axisymmetric Calculations for an LTV Aerobrake

Calculations are carried out for an LTV aerobrake to determine the effect of the new steric factor on the heat transfer rates in comparison to the conventional model. A typical point in this vehicle's trajectory during its return to Earth is at 100 km with a velocity of 7.95 km/s. The LTV under consideration by NASA-Marshall is a 70 deg, spherically blunt cone, with a R_n of 3.048 m and a base of 13.7 m. The Knudsen number λ_∞/l is 1.3 if l is the boundary layer thickness and 0.043 if l is the nose radius. This set of conditions characterizes a flow which is well within the transitional flow regime. Figure 7 shows the grid used for the computations.

The following reactions are used in this investigation:

1) $O_2 + O \rightarrow 2O + O$
2) $O_2 + N \rightarrow 2O + N$
3) $O_2 + O_2 \rightarrow 2O + O_2$
4) $O_2 + NO \rightarrow 2O + NO$
5) $O_2 + N_2 \rightarrow 2O + N_2$
6) $NO + O \rightarrow N + O + O$
7) $NO + N \rightarrow N + O + N$
8) $NO + O_2 \rightarrow N + O + O_2$
9) $NO + NO \rightarrow N + O + NO$
10) $NO + N_2 \rightarrow N + O + N_2$
11) $N_2 + O \rightarrow 2N + O$
12) $N_2 + N \rightarrow 2N + N$
13) $N_2 + O_2 \rightarrow 2N + O_2$
14) $N_2 + NO \rightarrow 2N + NO$
15) $N_2 + N_2 \rightarrow 2N + N_2$
16) $NO + O \rightarrow O_2 + N$
17) $N_2 + O \rightarrow NO + N$
18) $O_2 + N \rightarrow NO + O$
19) $NO + N \rightarrow N_2 + O$
20) $O + O + M \rightarrow O_2 + M$
21) $N + N + M \rightarrow N_2 + M$
22) $N + N + N \rightarrow N_2 + N$
23) $N + O + M \rightarrow NO + M$

where M is any other species present. Table 3 gives the rate constants and ϕ if applicable.

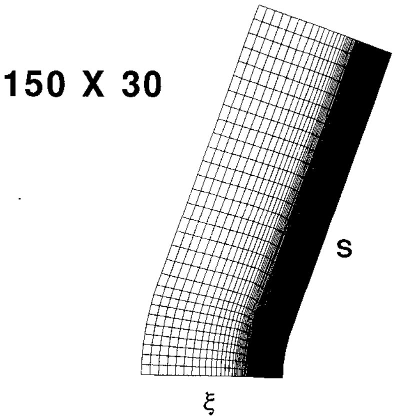

Fig. 7 Grid employed for 70-deg blunt cone with R_n = 3.048 m.

Table 3 Reaction set for LTV calculations

Reaction	A	α	E_a/k	ϕ
1	1.38×10^{-10}	-1.0	59,370	0.0
2	1.38×10^{-10}	-1.0	59,370	0.0
3	4.58×10^{-11}	-1.0	59,370	0.206
4	4.58×10^{-11}	-1.0	59,370	1.162
5	4.58×10^{-11}	-1.0	59,370	1.204
6	1.32×10^{-8}	-1.5	75,550	0.719
7	1.32×10^{-8}	-1.5	75,550	0.812
8	6.59×10^{-10}	-1.5	75,550	11.34
9	1.32×10^{-8}	-1.5	75,550	0.331
10	6.59×10^{-10}	-1.5	75,550	11.62
11	1.85×10^{-8}	-1.6	113,000	3.044
12	1.85×10^{-8}	-1.6	113,000	3.235
13	6.17×10^{-9}	-1.6	113,000	8.01
14	6.17×10^{-9}	-1.6	113,000	8.091
15	6.17×10^{-9}	-1.6	113,000	5.249
16	3.6×10^{-22}	1.29	19,700	——
17	5.3×10^{-17}	0.1	37,500	——
18	5.2×10^{-22}	1.29	3,600	——
19	2.02×10^{-17}	0.1	0	——
20	8.3×10^{-45}	-0.5	0	——
21	3.0×10^{-44}	-0.5	0	——
22	6.4×10^{-40}	-1.5	0	——
23	2.79×10^{-40}	-1.5	0	——

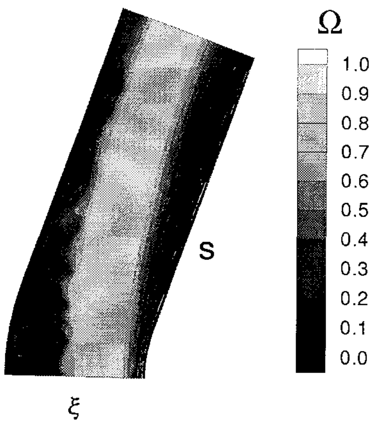

Fig. 8 Degree of vibrational nonequilibrium for the conventional model.

The dissociation rates, with the exception of the dissociation of NO, are from Park and Menes.[15] The rates for the dissociation of NO, the exchange reactions, and the recombination reactions are from Vincenti and Krueger.[20] The steric factors for exchange and recombination reactions in the new model are determined using the conventional method. The Park and Menes rates are widely used in DSMC simulations. Thus, we had to balance this fact with the fact that ϕ had to be set equal to zero for the O_2 + O and the O_2 + N reactions. We decided to live with the inconsistency instead of using a different set of reactions, because of the smaller frequency of such reactions for the conditions under consideration. It should be noted that use of Park et al. rates for O_2 + O and O_2 + N reactions results in values of ϕ which are 0.1 and 0.163, respectively.

Figures 8 and 9 shows contours of the degree of vibrational nonequilibrium for the LTV under consideration. This is measured with the parameter Ω where

$$\Omega = 1 - (T_v/T_t) \tag{24}$$

Nonequilibrium will correspond to values of Ω close to one, and equilibrium corresponds to values close to zero. In the figures, the dark regions are in thermal equilibrium and the gray regions are in thermal nonequilibrium. It is observed that the present model gives an increased region of nonequilibrium with a larger departure from equilibrium. Since dissociation is an important mechanism of internal energy exchange and relaxation, the delay of this mechanism results in a larger equilibrium departure.

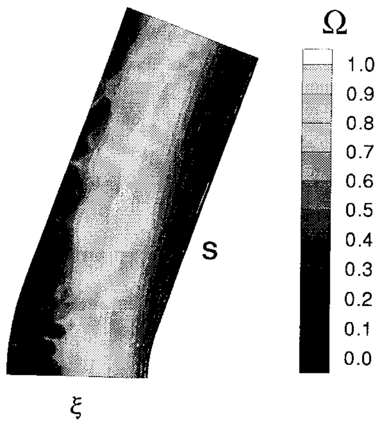

Fig. 9 Degree of vibrational nonequilibrium for present model.

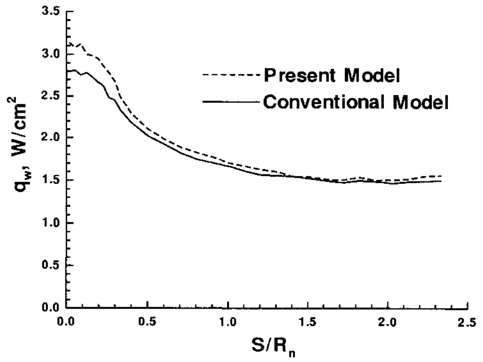

Fig. 10 Heat transfer rate along surface.

Figure 10 shows the heat transfer rates to the surface of the LTV for the two methods. The catalytic recombination coefficient is assumed to be 2%. The present model, which accounts for the effects of vibrational nonequilibrium, results in reduced dissociation and thus a larger heat transfer rate in the stagnation region. Differences in the heat transfer rate disappear away from the stagnation point because of the reduced vibrational nonequilibrium. The reason for this can be seen from Figs. 8 and 9 where equilibrium in both is achieved away from the stagnation region. Thus, if the peak heating of the aerobrake were to occur at a point in its trajectory for which significant thermal nonequilibrium was present, the design of the aerobrake should take into account vibration-dissociation coupling. This is because such coupling can have a significant effect on the heat transfer rates.

Concluding Remarks

Vibration-dissociation coupling has a significant effect on postshock properties. The present model provides a means to account for this coupling. The dissociation steric factor is bounded as the vibrational energy approaches the dissociation limit, can be used for gas mixtures, and does not appeal to experiment for determination of model exponents.

Vibration-dissociation coupling was seen to have a somewhat important effect on the stagnation region heat transfer rates to the surface of an LTV. The vibrational nonequilibrium delays the dissociation process such that less energy is removed by dissociation and more energy is imparted to the surface. Thus, modeling of vibration-dissociation is necessary to produce accurate estimations for stagnation region heat transfer rates for aerobrakes encountering flows characterized by thermal nonequilibrium.

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