Numerical Analysis of Relaxation Flows behind Extremely Strong Air Shock Waves

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The governing equations for a relaxation region behind strong shock waves were presented based upon a four-temperature flow model and were solved numerically as a one-dimensional analysis of a two-boundary value problem. The transport properties for viscosity, diffusion, and thermal conductivity were taken into account in detail, because flow and thermal conditions just behind shock fronts were expected to vary steeply. The change of vibrational and rotational energies of molecules, and free-electron energy due to dissociation and recombination reaction of diatomic molecules were also included. The rotational and vibrational temperature distributions calculated agreed very well with the experiments of ISAS/JAXA, indicating that the physico-chemical model used in the present analysis was valid.

1. Introduction

Research on relaxation phenomena behind strong shock waves is important because it is closely related to high enthalpy flow, reentry engineering, high-temperature gas radiation, and so on. Fundamental characteristics of the flows are determined by intense reactions in the relaxation region. Therefore, it is necessary to consider reaction systems as realistically as possible. As the thermal and fluid-dynamic quantities change steeply in this flow region, it is desirable to consider transport phenomena depending on the change rate of the valuables. A new model for energy changes of vibrational, rotational, and free-electrons due to dissociation and recombination reactions of diatomic molecules was presented by one of the authors3). Including these effects, a full set of governing equations based upon a four-temperature model for one-dimensional shock wave was presented, and was analyzed as a two-boundary value problem for the experimental flow conditions of ISAS/JAXA (Institute of Space and Astrophysical Science, Japan Aerospace Exploration Agency) of shock Mach numbers of 28, 36, and 37.73). Numerical results for molecular vibrational and rotational temperatures were in good agreement with the experiments, and it was found the flow model used in the present analysis was valid.

2. Basic Assumptions

The following assumptions are adopted.
(a) The flow is one-dimensional and in the steady state.
(b) Chemical reaction model for air is based upon 11 chemical species (N₂, O₂, NO, N, O, N₂⁺, O₂⁺, NO⁺, N⁺, O⁺, and e⁺) model with 33 chemical reactions.
(c) Temperature model is based upon 4-temperature model (heavy particle translational temperature \( T_o \), molecular rotational temperature \( T_r \), vibrational temperature \( T_v \), and free-electron temperature \( T_e \)). Temperature \( T_o \) is common to all heavy particles, and \( T_r \) and \( T_v \) to all molecules.
(d) Kinetic energies for all species are Maxwellian with \( T_o \) for heavy particles and with \( T_e \) for free-electrons. Population distribution over rotational levels is in Boltzmann distribution with \( T_r \), and
that over vibrational levels in Boltzmann distribution with $T_v$.

(e) The effects of radiation energy loss, precursor, and charge separation are neglected.

3. Governing Equations

Basic equations for one-dimensional relaxation flow behind strong shock waves were obtained by modifying the general equations for AOTV (Aeroassisted Orbital Transfer Vehicle) given by Lee$^1$ and by expanding them to the 4-temperature model. Coordinate system fixed on shock wave is adopted, and $x$-axis is taken from shock front along flow direction.

Conservation equation for total mass:

$$\frac{d}{dx} (\rho u) = 0$$

(1)

Conservation equation for total momentum:

$$\frac{d}{dx} (\rho u^2 + p) = \frac{d}{dx} \left( \frac{4}{3} \mu \frac{du}{dx} \right)$$

(2)

Conservation equation for chemical species:

$$\frac{d}{dx} (\rho u Y_s) = \frac{d}{dx} \left( \frac{\rho}{N m_i} D_s \frac{dy_{s}}{dx} \right) + \dot{w}_{s}$$

(3)

Conservation equation for total energy:

$$\frac{d}{dx} (\rho u H) = \frac{d}{dx} \left( \frac{4}{3} \mu \frac{du}{dx} \right) + \frac{d}{dx} \left( \eta_T \frac{dT}{dx} + \eta_r \frac{dT_r}{dx} + \eta_v \frac{dT_v}{dx} + \eta_e \frac{dT_e}{dx} \right)$$

$$+ \frac{d}{dx} \left( \sum_{i=1}^{10} \rho h_i D_i \frac{dy_i}{dx} \right)$$

(4)

Conservation equation for rotational energy:

$$\frac{d}{dx} (\rho u e_r) = \frac{d}{dx} \left( \eta'_T \frac{dT}{dx} \right) + \frac{d}{dx} \left( \rho \sum e_r D \frac{dy}{dx} \right) + \dot{Q}_r$$

(5)

Conservation equation for vibrational energy:

$$\frac{d}{dx} (\rho u e_v) = \frac{d}{dx} \left( \eta_v' \frac{dT_v}{dx} \right) + \frac{d}{dx} \left( \rho \sum e_v D \frac{dy}{dx} \right) + \dot{Q}_v$$

(6)

Conservation equation for free-electron energy:

$$\frac{d}{dx} \left( \frac{3}{2} N \rho \gamma \frac{k T_e u}{u} \right) = \frac{d}{dx} \left( \eta'_T \frac{dT}{dx} \right) + \frac{d}{dx} \left( \frac{5kT_e}{2m_e} \rho D_e \frac{dy_e}{dx} \right) + \dot{Q}_e$$

(7)

Equation of state:

$$p = \sum_{i=1}^{10} n_i k T_s + n_e k T_e = N \rho \left( \sum_{i=1}^{10} \gamma_i k T_s + \gamma_e k T_e \right)$$

(8)

In these equations, $\rho$ is the density of the fluid, $u$ the velocity, $p$ the pressure, $T$ the temperature, $\mu$ the diffusion coefficient of viscosity, $\gamma$ and $\gamma_e$ the mole concentration and mole fraction, respectively, $D_i$ the diffusion coefficient, $N$ the Avogadro's number, $k$ the Boltzmann constant, $m$ the mass, $H_i$ the total enthalpy, $\eta$ the thermal conductivity due to collisions between molecules and all particles, $\eta'$ the thermal conductivity due to collisions between the same kind of chemical species, $h_i$ the static enthalpy, $e_i$ the energy per unit mass, and the suffixes $u$, $r$, $v$, $e$, $M$ and $s$ means translation, rotation, vibration, electron, molecule, and chemical species $s$, respectively. In Eqs.(1)-(8), the terms on the left hand is a convective
Table 1 Coefficients for $D_e$

<table>
<thead>
<tr>
<th>Molecule</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>$d$</th>
<th>$e$</th>
<th>$f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N₂</td>
<td>-7.29576E-4</td>
<td>8.23373E-3</td>
<td>-0.0234288</td>
<td>0.0320843</td>
<td>-0.8248</td>
<td>9.7563</td>
</tr>
<tr>
<td>O₂</td>
<td>1.42473E-3</td>
<td>-0.021581</td>
<td>0.112221</td>
<td>-0.147154</td>
<td>-0.72701</td>
<td>5.1153</td>
</tr>
<tr>
<td>NO</td>
<td>4.25521E-4</td>
<td>-0.0087736</td>
<td>0.0601619</td>
<td>-0.0926535</td>
<td>-0.75229</td>
<td>6.4914</td>
</tr>
</tbody>
</table>

4.25521E-4 means $4.25521 \times 10^{-4}$.

term, and these on the right hand include transport and source terms ($\omega_x$, $Q_x$, $Q_y$, and $Q_z$) are contained.

4. Source Terms

The source terms in the conservation equations for chemical species directly depend on the model of chemical reactions. We considered dissociation and recombination reactions, exchange reactions, associative ionization reaction, and electron-impact reactions. For the chemical reaction rate constants for these reactions, basically, the Park's model\(^3\) was applied. However, for the dissociation and recombination reactions of diatomic molecules which were the most important reactions, the effective bond energy model of Jaffe\(^3\) was employed, because the present study was a 4-temperature analysis, and therefore Park's model based on two temperatures, namely translational and vibrational temperatures, was not directly applicable.

4.1 Effective Bond Energy of Molecules

Figure 1 shows the potential energy of N₂ molecule for three rotational quantum number $j=50$, 140, and 200. This figure was obtained by combining the R-K-R and H-H methods\(^3\). Figure 1 also shows the vibrational and rotational energy as $E_v$ and $E_j$ for state $(\nu, j)$. It is seen that, as molecule's rotational energy is increased, the contribution from the centrifugal terms results in the formation of a rotational barrier at a long range and effectively lowers the dissociation energy. The dissociation energy is $D_e$, as shown in the Fig. 1, for molecules at the rotational level $j$ and the vibrational level $\nu=0$. The effective bond energy $D_e$ can be calculated as a function of $T_r$ by averaging $D_i$ for all possible rotational levels weighted by a Boltzmann factor with $T_r$. The averaging was conducted for $j=0$ to $j_{\text{max}}$. The maximum rotational quantum number $j_{\text{max}}$ was determined from the fact that at rotational level of $j > j_{\text{max}}$, molecule cannot be formed because the potential well does not exist. $j_{\text{max}}$ for main air molecules N₂, O₂, and NO were 261, 225, and 233, respectively. $D_i$'s for these molecules thus calculated were plotted as a function of $T_r$ in Fig. 2. In this paper, $D_e$ was approximated by the following polynomials,

$$D_e(T_r) [\text{eV}] = at^3 + bt^2 + ct + dt^2 + et + f$$  (9)
where $t = T / 10,000$. This polynomials are applicable to $T = 50,000K$. The coefficients $a$, $b$, $c$, $d$, $e$, and $f$ for these molecules are shown in Table 1.

### 4.2 Dissociation and Recombination Rate Constants

Jaffe\(^{3}\) gave a following collision cross section for dissociation from state $(\nu, j)$ of a molecule due to collisions of a third body $M$,

$$\sigma_{\nu, j, M} = \sigma_{0M} \left(1 - \frac{E_{\nu, j}}{E}\right) \text{ for } E > E_{\nu, j},$$

$$\sigma_{\nu, j, M} = 0 \quad \text{for } E \leq E_{\nu, j},$$

where $\nu$ is the vibrational quantum number, $j$ the rotational one, $E$ the collision energy, $E_{\nu, j}$ the energy needed to dissociate from state $(\nu, j)$, and approximately given by $E_{\nu, j} = D_\nu - E_\nu$ using the above-mentioned $D_\nu$ and $E_\nu$. $\sigma_{0M}$ is the numerical factor which is assumed to be independent of $\nu$ and $j$, but depends on $M$. Using this cross section, the dissociation rate constant from the state $(\nu, j)$ is given as

$$k_{\nu, j, M} = \int_{E_{\nu, j}}^{\infty} F(E)\sigma_{\nu, j, M}(E)\nu(E)dE$$

by definition, where $F(E)$ is the distribution function for collision energy, assumed usually to be Maxwellian, $\nu(E)$ the collision velocity. Total dissociation rate coefficient for collisions of $M$ is obtained by $\sum_{\nu} \sum_{j} k_{\nu, j, M}$, resulting in\(^{3}\),

$$k_{\nu}(T_w, T_v, T_e) = \frac{8kT_v}{\pi M} \sigma_{0M} \left(\frac{T_w}{T_w - T_v}\right) \frac{\exp\left(-\frac{D_\nu}{kT_v}\right) - \exp\left(-\frac{D_\nu}{kT_w}\right)}{1 - \exp\left(-\frac{D_\nu}{kT_v}\right)}$$

where $\sigma_{0M}$ can be determined by the comparison with the rate constant of the Park's model\(^{3}\) based on experiments in assuming the thermal equilibrium state, and if the third body is electron, $T_w$ is replaced by $T_e$.

### 4.3 Source Terms in the Conservation Equations

The source terms in the vibrational, rotational, and free-electron energy equations are given by, respectively,

$$\dot{Q}_\nu = Q_{\nu, R} - Q_{\nu, 0},$$

$$\dot{Q}_v = Q_{v, \nu} + Q_{v, \nu} - Q_{\nu, 0},$$

$$\dot{Q}_e = Q_{e, 0} + Q_{e, 0} - Q_{\nu, 0},$$

where $Q_{\nu, R}$ is the energy exchange rate between heavy particle's translation and molecular rotation, $Q_{\nu, \nu}$ the rate between heavy particle's translation and molecular vibration relaxation term, $Q_{v, \nu}$ the rate between electron and molecular vibration, $Q_{\nu, el}$ that due to elastic collisions, and $Q_{\nu, el}$ that due to inelastic collisions. A model for the electron-rotation energy exchange is available for $N_2$, $O_2$, and NO. However, this is not commonly used and this mechanism is assumed to be negligible in this work. The terms $Q_{\nu, 0}$, $Q_{e, 0}$, and $Q_{e, 0}$, based upon Shirai's model\(^{3, 2}\), are the net energy losses of rotation, vibration, and free-electron, respectively, due to dissociation and recombination reactions. For the terms $Q_{\nu, R}$ and $Q_{v, \nu}$, the diffusion model developed by Park\(^{3}\) and Lee\(^{3}\) was adopted, respectively, and for $Q_{\nu, 0}$ the same model by Lumpkin\(^{10}\) was adopted.

### 5. Boundary Conditions and Calculation

The governing equations were normalized by the equilibrium conditions and the calculated distance. A set of parabolic differential equations obtained was solved numerically for air by the successive
accelerated replacement (SAR) method as a two-boundary value problem. The present calculations were conducted for the flow conditions of ISAS/JAXA experiments, namely, air shock Mach number of 36 and 37.7, and initial pressure 0.3 Torr, and in case of the shock Mach number 28, initial pressure was 2.1 Torr. Then, Initial distributions of various flow and thermal parameters were given by solving the governing equations without the transport terms, the rotational energy equation, and the net energy losses due to dissociation and recombination reactions by the Runge-Kutta-Gill method as an initial value problem. The boundary values were set to be the same as equilibrium values at a far distance downstream, and the Rankine-Hugoniot relations for the parameters except \( T_r \) and \( T_v \), which were assumed to be low and arbitrarily selected, at just behind shock front. The transport coefficients \( \mu, \eta, \eta', \) and \( D_r \) were taken from Yos. Calculation distance behind shock front was 0.1 m for these shock speeds, and divided into equal 1,000 steps.

6. Results and Discussion

Figures 3 and 4 show the distribution of the temperature and chemical species' mole fraction, respectively, for shock Mach number \( M_r = 36 \), initial pressure \( p_i = 0.3 \) Torr, and initial temperature 300 K. In Fig. 3, experiments of ISAS/JAXA were also shown with the result based on Park's model, which was calculated by ISAS/JAXA researchers. The solid lines are the present analysis, and the dashed lines are the Park's model. For the experimental data of ISAS/JAXA, the solid triangle and circle mean \( T_r \) and \( T_v \) determined by applying a spectral matching method to the spontaneous emissions of the \( N_2^+ \), and the opened symbols to those of the \( N_2 \). It is apparent that, in the present calculation, the temperatures were remarkably different from each other in the entire relaxation region, indicating the extremely nonequilibrium state. As compared with the results of Park's model, the behavior of the rotational temperature was much different from it, and the relaxation distance was much shorter than that. In the present calculation, the vibrational and rotational temperatures were assumed to be same for all molecules. Therefore, it was impossible to compare the \( T_r \) and \( T_v \) of \( N_2^+ \) and \( N_2 \), individually, with the experiments for each molecule. In the relaxation zone except the just behind shock front, the concentration of \( N_2^+ \) molecule is much higher.
than $N_2$, $N_2^+$ molecules had most of the vibrational and rotational energies included in the plasma. From the point of this view, it can be said that the present results for $T_v$ and $T_r$ were in good agreement with experiments. In Fig.5, similar results to the above were shown for the conditions of shock Mach number 37.7, initial pressure 0.3Torr, and initial temperature 300K. In this case, too, the calculated and experimental results were agreed very well, and the physico-chemical model adopted in the present analysis was very realistic. In the final stage of the relaxation, the region, in which the $T_v$ and $T_r$ were very high, was appeared. It is apparent that this was caused the molecular recombination, as seen from the distribution of $N_2$ and NO in Fig. 4, for which the chemical energy was released and transferred to molecular vibrational and rotational energy modes. The appearance of this phenomenon was significantly dependent on shock Mach number, as seen from the comparison of Figs. 3 and 5. In case of shock Mach number below 30, this phenomenon would be disappeared.

This analysis gave a remarkably short relaxation distance as compared with the model of Park. This caused mainly by a difference between the dissociation and recombination rate constants used. Temperature difference between the present and Park's model, particularly the difference in the rotational temperature was owing to the difference of the model associated with the energy changes of molecular vibrational and rotational energy modes, and free-electron energy due to the chemical reactions. Agreement between the present analysis and the experiment of vibrational and rotational temperatures may show that the physico-chemical model proposed by one of the authors is valid.

7. Conclusions

A set of basic equations governing the shock wave flows was given. In the equation system, dissociation model proposed by Jaffe and the energy change of molecular vibrational and rotational energy modes, and free-electron energy due to dissociation and recombination reactions by Shirai were adopted. Numerical analysis was conducted by the SAR method as a two-point boundary value problem, in which various transport terms were taken into account. The numerical results for the temperatures $T_v$, $T_r$, and $T_T$ agreed very well with the experiments of ISAS/JAXA, and the physico-chemical model used in the present analysis was valid.

References