A Thermochemical Nonequilibrium Flow around a Super Orbital Reentry Capsule

Ryoji Doihara and Michio Nishida

Department of Aeronautics and Astronautics, Kyushu University, Fukuoka 812-8581, Japan

Abstract. The aerodynamic heating to the super orbital reentry capsule of MUSES-C is numerically studied by using thermochemical nonequilibrium full Viscous-Shock-Layer (VSL) equations. An 11 air-species model is used for non-ablating boundary conditions. Six carbonous species are added for ablating boundary conditions. With a three-temperature model, thermal nonequilibrium effect is taken into account. The convective and radiative heat fluxes to the wall are examined for both fully catalytic wall (FCW) condition and non-catalytic wall (NCW) condition at various altitudes for the capsule reentry trajectory path. The maximum heat fluxes estimated for FCW and NCW are 8.7 MW/m$^2$ at the altitude of 56 km and 6.1 MW/m$^2$ at the altitude of 56 km, respectively. The radiative heat flux at the stagnation point of the capsule has also been calculated and the maximum radiative heat flux of 0.9 MW/m$^2$ has been found at the altitude of 62 km. The intensity of UV and VUV spectra are extremely intense, so that such UV and VUV spectra mainly contribute to the radiative heat flux.

INTRODUCTION

The asteroid sample return mission “MUSES-C” is being prepared at the Institute of Space and Astronautical Science [1]. In this project the capsule which transports samples from the asteroid is to enter into the earth’s atmosphere directly from the hyperbolic earth-return trajectory. The atmospheric entry speed of the capsule is over 12 km/s, so that a very strong shock wave is generated around the capsule, whereby the shock layer gas is much more highly heated than the case of a normal earth orbital reentry. Hence, it is predicted that radiative heat flux will be stronger in the super orbital reentry than in the earth orbital reentry. To make the effective design of the thermal protection system within the tightly limited weight, it is important to make more accurate estimation of aerodynamic heating and to reveal the degree of the contribution of the radiative heat flux.

A strong shock wave causes molecules of atmosphere to be dissociated and ionized, and consequently the shock layer gas will consist of molecules, atoms, ions and electrons. Density of air is quite low at high altitudes where characteristic times of chemical reactions and energy exchange will be of comparable order with the characteristic time of the flow or more. Therefore, this flow field will be in thermochemical nonequilibrium. Under these conditions, translational, rotational, vibrational, electron and electronic temperatures are not essentially equal. Therefore, in order to analyze such a reentry flow field, thermochemical nonequilibrium cannot be avoided.

In this study the numerical analysis of the shock layer flow over the super orbital reentry capsule has been performed by using the thermochemical nonequilibrium viscous shock layer (VSL) equations. The VSL equations have been often used in order to analyze the nonequilibrium flow over a hypersonic body [2]- [4]. Of these, Ref. [4] is cited as the work treating a super-orbital reentry. In Ref. [4], the flowfield over the MUSES-C capsule was analyzed using a two-temperature model consisting translational-rotational and vibrational-electron temperatures, and heat fluxes to the wall for FCW and NCW were discussed. In case of the super orbital reentry, radiative heat flux on the wall cannot be neglected. Intensity of radiation is strongly dependent on vibrational, electron and electronic temperatures, so that the temperature nonequilibrium should be calculated more accurately. The MUSES-C capsule will have a heat shield made of C/C composite material. The carbonous species will be ablated from the surface of the heat shield and may influence radiative heat flux. For this reason, a three-temperature model in which translational-rotational, vibrational and electron-electronic...
temperatures are treated as different from each other will be an adequate temperature model. To consider the effect of ablating species, 19 reactions of 6 carbonous species are added to the 11 air species model.

The present paper is concerned with the numerical analysis of the flow field over the super-orbital reentry capsule. The analysis uses a three temperature model for the reason mentioned above and nonequilibrium air chemistry is represented by using an 11 air species model and 6 carbonous species model. Furthermore radiative heat flux to the wall is estimated using SPRADIAN which is the computational code for estimating spectral intensity and radiative heat flux developed by Fujita and Abe [5]. Tauber et al. proposed a simple formula for reentry aerodynamic heating [6], which assumed that the vehicle surface is fully catalytic to atomic and molecular recombinations. Tauber and Sutton also proposed a simple formula for radiative heat flux [7]. It also is one of the present purposes to examine the applicability of these simple formulas to the super-orbital reentry problem.

METHOD OF ANALYSIS

A Governing equations

The governing equations are the VSL equations formulated for a multicomponent gas flow in thermochemical nonequilibrium. The VSL equations are obtained from the steady-state Navier-Stokes equations by retaining terms up to the second order in the Reynolds number parameter $\epsilon$ defined by $\epsilon = \sqrt{\mu_\infty / \rho_\infty U_\infty R_n}$ where $\mu_\infty$ is the viscosity at the free stream temperature, $\rho_\infty$ the free stream density, $U_\infty$ the free stream speed and $R_n$ the nose radius of a body. In the present study, the value of $\epsilon^3$ is in the order of $10^{-2}$ to $10^{-4}$, so that the VSL analysis is expected to provide sufficiently accurate solutions.

The configuration of the reentry capsule is given by a hyperboloid with 20 cm in the nose radius and 45 deg in the semi-apex angle.

B Transport properties

For the 11-species model, the transport properties are evaluated by extending Yos’ formula, which is based on the first Chapman-Enskog approximation, to the multi-temperature gas mixture [8]. For ablation analysis, the viscosity and thermal conductivity for a mixture of gas are computed using Wilke’s semi-empirical formula and Yos’s formula. The viscosities of the species are calculated from the curve fit form of Blottner [9]. Curve fit data for the species are used in Ref. [10]. The diffusion coefficients of Curtiss and Hirschfelder [11] are used. For ions, ambipolar diffusion is assumed.

C Energy exchange

The energy transfer rate between translation and vibration is derived from the formula of the Landau-Teller model. The vibrational relaxation time is evaluated by an empirical formula of Millikan and White [12] involving the correction term of Park’s collision limit [13]. The translation-electron and rotation-electron energy transfer rates are taken from Lee [14], and Lazdinis and Prtrie [15], respectively. In the energy exchange between vibrational and electron modes, only the vibrational energy of nitrogen is considered because the nitrogen-electron coupling is much stronger than others. The relaxation time of this exchange is taken from Lee [16]. The average vibrational energy removed by dissociation is assumed to be 50 % of dissociation energy.

D Air chemistry

In the case of the super orbital reentry, the temperature behind a shock exceeds 50,000 K. Molecules are fully excited at vibrational energy levels. At the same time these molecules dissociate into atoms and ionize into ions, so that we use an 11 species air (76.5 % N$_2$ + 23.5 % O$_2$ in the freestream) model consisting of N$_2$, O$_2$, NO, N, O, NO$^+$, O$^+$, N$^+$, N$_2^+$, O$_2^+$ and e$^-$. We consider 48 chemical reactions of these 11 species given in Table 1. The chemical reaction rate model is the Park model [13] that uses effective temperature extended
to a three temperature model. Reaction rates are assumed to be a function of controlling temperatures $T_i$ and $T_b$, depending on the type of reaction, and they are given by the following expressions:

$$k_{t,r}(T_{i,r}) = C_{r,s} \exp(-\theta_r/T_{i,r})$$

(1)

$$k_{b,r}(T_{b,r}) = k_{t,r}(T_{b,r})/K_{r,s}^{\theta_r}(T_{b,r})$$

(2)

The controlling temperatures are shown in Table 1. The values of $C_{r,s}$, $s_r$ and $\theta_r$ are obtained from Ref. [13]. For the ablation analysis, 19 chemical reactions of 6 carbon containing species are added to the 11 air species. The reaction rates of 19 reactions are from Blottner [9] and shown in Table 2.

\[ \begin{array}{c|c|c|c} \hline r & \text{Reactants} & \text{Products} & \hline \hline 1 & N_2 + M_i & \equiv N + N + M_1 & \sqrt{T - T_{\text{vib}}} T \\
2 & N_2 + M_k & \equiv N + N + M_2 & \sqrt{T - T_{\text{vib}}} T \\
3 & N_2 + e^- & \equiv N + N + e^- & \sqrt{T - T_{\text{vib}}} T \sqrt{T - T_e} \\
4 & O_2 + M_i & \equiv O + O + M_1 & \sqrt{T - T_{\text{vib}}} T \\
5 & O_2 + M_k & \equiv O + O + M_2 & \sqrt{T - T_{\text{vib}}} T \\
6 & NO + M_i & \equiv N + O + M_1 & \sqrt{T - T_{\text{vib}}} T \\
7 & NO + M_k & \equiv N + O + M_2 & \sqrt{T - T_{\text{vib}}} T \\
8 & N_2 + O & \equiv NO + N & T T \\
9 & NO + O & \equiv N + O_2 & T T \\
10 & N + O & \equiv NO^* + e^- & T T \\
11 & N + N & \equiv N_2^* + e^- & T T \\
12 & O + O & \equiv O^*_2 + e^- & T T \\
13 & NO^* + O & \equiv N^* + O_2 & T T \\
14 & O_2^* + N & \equiv N^* + O_2 & T T \\
15 & NO^* + O^* & \equiv N^* + O_2 & T T \\
16 & O_2^* + N_2 & \equiv N_2^* + O_2 & T T \\
17 & O_2^* + O & \equiv O^* + O_2 & T T \\
18 & NO^* + N & \equiv O^* + N_2 & T T \\
19 & NO^* + O_2 & \equiv O^*_2 + NO & T T \\
20 & NO^* + O & \equiv O^*_2 + N & T T \\
21 & O^* + N_2 & \equiv N^*_2 + O & T T \\
22 & NO^* + N & \equiv N^*_2 + O & T T \\
23 & N + e^- & \equiv N^* + e^- + e^- & T_e T_e \\
24 & O + e^- & \equiv O^* + e^- + e^- & T_e T_e \\
\hline \end{array} \]

\[ ^aM_i = N_2, O_2, NO, N_2^*, O_2^*, NO^+ \]

\[ ^bM_k = N, O, N^+, O^+ \]

\[ ^cM_3 = N_2, O_2, N_2^*, O_2^* \]

\[ ^dM_4 = NO, N, O, NO^+, N^+, O^+ \]

**TABLE 1.** Chemical reactions of 11 air species

**TABLE 2.** Chemical reactions of 6 carbon-containing species

E Solution procedure

In the VSL analysis, the equations of tangential-momentum, translational-rotational energy, vibrational energy, electron-electronic energy and species conservation are written in the same standard parabolic form as Ref. [17]. These equations are rewritten in a tridiagonal matrix by using a second order finite difference method. The tridiagonal matrix is easily solved using Thomas algorithm. However in this study, numerical instabilities occur in overall iteration of these equations because of the usage of a three temperature model. To avoid this, a relaxation term $(W^{k+1} - W^k)/\Delta$ is added to the standard parabolic form:

$$\frac{W^{k+1} - W^k}{\Delta} = \frac{\partial^2 W^{k+1}}{\partial \eta^2} + A_1 \frac{\partial W^{k+1}}{\partial \eta} + A_2 W^{k+1} + A_3 + A_4 \frac{\partial W^{k+1}}{\partial \xi},$$

(3)

where $k$ is the iteration number, $\Delta$ is the relaxation parameter, $W$ represents the normalized physical value of $u, T, T_{\text{vib}}, T_e$ and $C$. If the number of iteration is sufficient for convergence of $W^{k+1} \rightarrow W^k$, this equation becomes the same as the standard parabolic equation. Using this method, the equations can be solved asymptotically. First, the VSL equations on the stagnation streamline are solved. Next, the downstream portion
is calculated by a space marching method where an initial shock profile is assumed to be parallel to a body surface. Then, shock layer properties are determined and the shock profile is refined. For the new shock profile, the VSL equations are newly solved iteratively until the shock layer properties do not change. In the present calculation, 101 grid points are put between the body and shock in the direction normal to the body.

F  Boundary conditions

At the wall, no-slip conditions \( (u = v = 0) \) are imposed. The species wall boundary conditions are determined by using either noncatalytic wall (NCW) condition \( \left( \partial C_i / \partial y \right)_w = 0 \) or fully catalytic wall (FCW) condition \( C_i = C_i^w \). The wall temperature \( T_w \) is assumed to be constant at 2,500 K in 11 air-species analysis. The vibrational temperature on the wall is equal to the wall temperature. The boundary condition of the electron temperature is calculated by Eq. (10) in Ref. [18] that is derived from the Langmuir probe theory. Boundary conditions immediately behind the shock are estimated from free stream conditions along with the reentry trajectory (Fig. 1) by shock jump conditions. To consider low density gas effect, shock boundary conditions are determined by using shock slip conditions [17]. Vibrational temperature and electron temperature are set to being equal to the freestream temperature.

For the ablation analysis, we consider the sublimation of C\(_3\) and the oxidation by atomic oxygen as ablating boundary conditions. The oxidation by O\(_2\) is not considered because the reaction probability is negligibly small in comparison with that by atomic oxygen. The O and CO mass fluxes due to oxidation are given as:

\[
J_{O,oxi} = -\rho_O K_{w,oxi} \quad J_{CO,oxi} = \frac{M_{CO}}{M_O} \rho_O K_{w,oxi}
\]

where

\[
K_{w,oxi} = \alpha \sqrt{\frac{RT_w}{2\pi M_O}}
\]

The reaction probability \( \alpha \) is given as follows [19]:

\[
\alpha = 0.63 \exp(-1160/T_w)
\]

The sublimation of C and C\(_2\) is not considered, since their equilibrium vapor pressure is much lower than that of C\(_3\). The mass flux due to sublimation of C\(_3\) is given by the Hertz-Knudsen-Langmuir relation [9]:

\[
J_{C_3,sub} = \frac{\alpha_{C_3} \cdot Max(0, P_{e,C_3} - P_{C_3})}{\sqrt{2\pi (R/M_{C_3}) T_w}}
\]

where \( P_{e,C_3} \) and \( P_{C_3} \) are equilibrium vapor pressure and partial pressure, respectively. The value of constants of \( \alpha_{C_3} \) and \( P_{e,C_3} \) are given in Ref. [9].

G  Radiation calculation

The VSL analysis is not coupled with the calculation of radiative heat transfer. Radiation analysis is performed by SPRADIUS [5] in non coupled manner, using flow field of stagnation stream line calculated by the VSL code. In the estimation of radiative heat flux, the spherical cap model [5] is used for the integration of the heat transfer equation.

RESULTS AND DISCUSSION

Figure 2 shows the convective and radiative heat transfers on the stagnation point against altitude in the 11 air species analysis. The line of Tauber et al. has been calculated based on Ref. [6]. The VSL result for the FCW condition shows the feature similar to the Tauber formula, which increases monotonously with decreasing altitude between the altitudes of 90 km and 58 km. The heat flux for the FCW is less than that predicted by the formula of Tauber et al. except for altitudes over 76 km and has a maximum of 8.7 MW/m\(^2\) at 56 km.
Hence, it can be seen that the formula of Tauber et al. overestimates the heat flux for FCW. The heat flux for NCW has the maximum of 6.1 MW/m² at the altitude of 56 km.

The radiative heat transfer becomes significant at the altitudes from 70 km to 55 km. At these altitudes, so-called avalanche ionization phenomenon [20] is seen and leads to larger electron density and temperature. As a result, radiative heating becomes strong. The maximum radiative heating is approximately 0.9 MW/m² at the altitude of 62 km. The difference between the radiative heat fluxes for NCW and FCW cannot be seen. The line of Tauber & Sutton denotes the radiative heat flux estimated for air based on Ref. [7]. The result of Tauber & Sutton also overestimates radiative heat flux compared with the present VSL result. The radiative heat flux evaluated from the calculated flow properties has the maximum of 0.9 MW/m² at the altitude of 62 km. UV and VUV spectra observed at the stagnation point are extremely large because of the disappearance of O₂ which absorbs such spectra.

Figures 3 and 4 illustrate the distribution of the mole fractions in the ablation analysis on the stagnation streamline (H = 64 km, Tₜₘₐₓ = 2,500 K, 19 species model). In all the ablation analyses, the species for air are assumed to be fully-catalytic condition. It can be seen that the degree of ionization becomes fairly high and dominant species are N, O, N⁺ and e⁻. The mole concentration of the electron increases in the region from 0.5 to 0.3 which is attributed to the electron-impact ionization (N + e⁻ → N⁺ + e⁻ + e⁻). The rate coefficient for this reaction is intrinsically large because of the high thermal speed of electrons. If electron temperature and density become over certain high values, this process occurs as a chain reaction. It is said that this phenomenon, called “Avalanche Ionization”, is one of the characteristics of a super orbital flight velocity [20]. At this wall temperature (Tₜₘₐₓ = 2,500 K), the oxidation is significant. The mole fractions of CO and C are large in these carbon containing species.

Figure 5 shows the mole fractions of carbonous species on the stagnation streamline in case that the wall temperature is 3,200 K. It is seen that the mol fraction of C₃ becomes large compared with the value in Fig.4. The sublimation of C₃ becomes significant. C₃ is rapidly dissociated into C₂ and C and these two species and air species recombined into CN and CO₂.

Figure 6 shows the variations of the stagnation heat flux with the wall temperature in the ablation analysis at the altitude of 64 km. At Tₜₘₐₓ = 2,500 K, the stagnation heat fluxes with and without ablation are almost equal. At the wall temperatures over 3,000 K where the sublimation becomes significant, the stagnation heat flux is rapidly reduced.

Figures 7 and 8 illustrate radiation spectra that is calculated by SPRADIAN [5] on the stagnation point at the altitude of 64 km (Tₜₘₐₓ = 3,200 K) with and without ablation, respectively. The strong emission line spectra from N, N⁺ and O are identified below 2,000 Å and over 7,000 Å. N₂⁺ (1-) and N₂⁺ (2+) band spectra are also observed in the range from 3,000 Å to 5,000 Å. The radiative heat flux without ablation is 0.86 MW/m². In the spectra with ablation, line spectra of C and band spectra of CN(Violet) and C₂(Swan) are observed. The radiative heat flux with ablation slightly increases to the value of 0.96 MW/m².
**FIGURE 3.** Mole fractions of air species on the stagnation streamline ($H=64$ km, $T_w=2,500$ K)

**FIGURE 4.** Mole fractions of carbonous species on the stagnation stream line ($H=64$ km, $T_w=2,500$ K)

**FIGURE 5.** Mole fractions of carbonous species on the stagnation stream line ($H=64$ km, $T_w=3,200$ K)

**FIGURE 6.** Variations of stagnation heat flux vs wall temperature

**FIGURE 7.** Radiation density at the stagnation point without ablation ($H=64$ km, $T_w=3,200$ K)
I
&
* «
I
8
1e+06
100000
10000
1000
100
10
1
0.1
N,0,N
N,0,N
Qr
ad
.=0.96MW/m².
CN(Violet) N,O,C
C²(Swan)
N,O,C(line)

FIGURE 8. Radiation density at the stagnation point with ablation (H=64 km, T_w=3,200 K)

CONCLUSION

The heat fluxes to the super orbital reentry capsule have been numerically analyzed by using the viscous shock layer equations with a three temperature model and nonequilibrium air chemistry. It has been found that the heat fluxes for FCW and NCW have the maximum of 8.7 MW/m² at the altitude of 56 km and 6.1 MW/m² at the altitude of 56 km in non-ablation analysis, respectively. The radiative heat flux evaluated from the calculated flow properties has the maximum of 0.9 MW/m² at the altitude of 62 km in non-ablation analysis. UV and VUV spectra observed at the stagnation point are extremely large because of the disappearance of O₂ which absorbs such spectra.

The ablation by the sublimation becomes significant at the wall temperature higher than 3,000 K and reduces the wall heat flux largely. When the wall temperature is low, the ablation occurs by the oxidation. However the wall heat flux is hardly reduced by the ablation due to oxidation. The ablation species slightly increase the radiative heat flux.

REFERENCES