High Enthalpy Flow Simulation with Ablation
Overview of Research for Prediction of Aerodynamic Heating Environment During a Super-Orbital Reentry Flight of MUSES-C Reentry Capsule

By

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To develop the heat shield system for the reentry capsule, the prediction of aerodynamic heating environment along the flight path is required. At the same time, the prediction of the response of the ablator-type heat shield is required. To meet these requirements, intensive research has been conducted.

The flow field around the MUSES-C reentry capsule is expected to be very complex in manyfolded way, because of its high speed reentry such as 12 km/sec unlike the reentry from LEO. Because of this complexity, we were able to foresee, from the beginning of the research phase, many difficulties which can be neglected for the reentry from LEO; 1) high energy chemical reactions such as ionization must be taken care of, 2) radiative heating must be taken care of, and 3) thermochemical nonequilibrium, which is unknown for the moment, may be influential.

To solve these problems, experimental studies are inevitable. Nevertheless, because of the limitation inherent to the experimental investigations and availability of the facility, much effort has been devoted to the numerical investigations, for the prediction of the aerodynamic heating environment. In addition to these phenomenological difficulties, other difficulties related to numerical technique, such as numerical instability, were foreseen because of its high speed reentry. For the thermochemical model, the Park’s two-temperature model (Park 1989) was employed as a basic model, even though the model was developed for application to the reentry smaller than the present speed reentry and thus several extensions were foreseen to be made, from the beginning. Otsu (1998) successfully solved the flow field around the MUSES-C reentry body, extending the original Park’s model and showing that the numerical difficulties can be avoided by employing AUSUM-DV scheme which is known as numerically tough scheme previously. In the simulation, the thermal quantities such as enthalpy above 30 thousands degrees kelvin, below which the data is published already, were required because of its high reentry speed. They are therefore modeled theoretically in the simulation. Other way to

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avoid the difficulty related to numerical instability is to solve the viscous shock layer equations which are approximate equations for the N-S equations, but can be applicable to the flow field prediction in a certain region of the flight path. Suzuki (1997; 2003), Nishida (2003) and Zulkov (1999) took this approach. As for the prediction of the convective heating rate at the front side, those results shows a reasonable agreement to each other.

For the numerical analysis, we employed the Park's model basically. However, there are several uncertainty and choices in the model such as diffusion coefficient (Otsu et al. 2001; Otsu 2003), and various thermal nonequilibriums. Since these phenomena are directly related to the heating rate, the influence of these uncertainties on the heating rate have been investigated. Otsu assess the effect of the different diffusion coefficients. The influence of the thermal nonequilibrium can be assessed since, in Nishida's analysis (2003), the electron temperature was treated independently from other translational and vibrational temperature. Compared to the results based on the two temperature model, the effect of this thermal nonequilibrium is not large. Other than this thermal nonequilibrium, the effect of rotational temperature nonequilibrium was assessed (Fujita et al. 2000). The non-equilibrium, which was neglected for the reentry from LEO, was suggested by the shock-tube experiment which will be mentioned later. Fortunately, the effect is not influential.

For the high-speed reentry, the radiative heating rate must be taken care of. To access the radiative heating based on the CFD prediction of the flow field, the data base for the radiation is required. For this purpose, we have developed the database “SPRADIAN” which is similar to the NEQAIR code (Fujita et al. 2003). Otsu (1998) made the prediction for the radiative heating rate based on SPRADIAN. The typical predicted values are slightly smaller than the simple prediction. Similar result was obtained by Sawada (2003) who calculated the radiative heating rate based on the data base different from SPRADAIN. The radiative heating becomes about 15% of the convective heating rate. In the analysis mentioned above, the radiative coupling with the flow field is ignored. For more precise prediction, the coupling analysis is necessary for a future task.

For the heat shield system for MUSES-C capsule, the ablator-type heat shield was employed for the heat protection system. For the evaluation of the ablator-type heat shield along the flight path, the prediction of bond line temperature and the total recession is required. For the development of the ablator system, however, the prediction of the aerodynamic heating rate with ablation effect is necessary. One of the effects caused by the ablator system is the effect of ablation gas mixing into the flow field. When the ablation gas mixes into the flow field, it influences not only on the convective heating rate but also on the optical properties of the flow field. Otsu (1999) predicted its effect on the radiative heating rate and shows that the radiative heating rate at the stagnation region rises slightly (approximately by 10%). Similar results were obtained by Nishida (2003). This is caused, largely by the radiation from C. On the aft-side, however, it rises by approximately 5 times, because of the ablation gas effect. In spite of this rise, the radiative heating rate on the aft-side remains to be about 1% of that of the front size. Another effect caused by the ablator system is the effect of the catalysis of the ablator surface. Zulkov (1999) estimated the effect of the catalysis of the carbon surface which is considered to be a replacement for the charred surface of the ablator. In spite of the theoretical investigations, there remains uncertainties of the extent of the catalysis effect of the charred ablator system.

As mentioned above, our analysis is based on the Park’s two temperature model. Even though the uncertainty in the prediction, which may be derived from the uncertainty in the thermochemical model, is assessed, the experimental validation is desirable. For this purpose,
we have carried out the shock tube experiment in which the flow field generated by the strong shock wave with the shock speed comparable to the flight velocity was investigated. In the experiment, various discrepancies are observed (Abe 2003; Fujita et al. 1998; 1999; 2001; 2001; Matsuda et al. 2002). One discrepancy is the nonequilibrium between rotational and translational temperatures which are assumed to be in equilibrium in the Park’s model. Another one is an abnormally high electron density behind the shock wave. The detailed mechanisms for these discrepancies are under investigation (Fujita et al. 2002). Beside the shock tube experiment, the expansion tube experiment was carried out to provide the high speed flow which corresponds to the flight speed of approximately 8.5 km/sec (Sasoh 2003). The shock standoff distance of the shock wave around the sub-scale model of the MUSES-C was measured and compared to the CFD result. The agreement between them is reasonable. For higher reentry speed, another result by means of the expansion tube was obtained by McIntyre (2001). According to Otsu (2002), the agreement between the numerical prediction and the experimental result is not good as was suggested by the discrepancy observed in the shock tube experiment. He suggested that the adjusting in the thermochemical model could explain the discrepancy. Again, for the higher speed reentry, much intensive work is still necessary.

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Chemical Nonequilibrium Viscous Shock-Layer Analysis over Ablating Surface of Superorbital Re-Entry Capsule

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Abstract: The aerodynamic heating environment with ablation injection and the mass loss rate of the ablator under the superorbital re-entry condition of the MUSES-C sample return capsule are numerically studied by solving the viscous shock-layer (VSL) equations with the nonequilibrium chemistry of both the air and the ablation gas. The boundary conditions at the ablator surface are formulated by considering the surface oxidation and surface sublimation. Computational results on the variation of the surface mass loss rate with the wall temperature demonstrate that the diffusion-controlled regime and the sublimation regime are successfully described by the present model. The time history of the wall temperature at the stagnation point is estimated along the re-entry trajectory by assuming the energy balance at the surface. The streamwise distributions of the convective heating rate and the surface mass loss rate over the forebody of the capsule are calculated at the peak heating flight condition and their characteristics are clarified. The effects of the pyrolysis gas of hydrocarbon species on the convective heating rate are investigated. The possibility of wall heating augmentation due to the turbulence induced by the ablation injection is also discussed.

1. INTRODUCTION

At the next step of the exploration on our solar system, the sample-return mission is expected to play an important role, since precise investigation of soil samples in laboratories leads us to much further understanding about planets, asteroids, comets and so on. For simplicity of the spacecraft system and reduction in the mission cost, it is necessary to establish the technology of the superorbital re-entry in which a small re-entry capsule carrying the sample of a target body enters the Earth’s atmosphere directly from the interplanetary trajectory at superorbital velocity to save the spacecraft fuel for orbit insertion. At the Institute of Space

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and Astronautical Science (ISAS), Japan, the asteroid sample return mission called "MUSES-C" (ISAS 1995) is in development aiming for launch in 2003. In this mission, a 20 kg small blunt cone capsule is used and its nominal entry velocity is 12.5 km/s at altitude 100 km.

To protect the payload from the severe aerodynamic heating of superorbital re-entry, the ablator of the carbon-phenolic type is planned to be used. The peak stagnation aerodynamic heating is expected to occur around 60 km altitude, where the shock layer flow is in fully chemical nonequilibrium. Consequently, for evaluation of the heat shield performance we must consider the chemical nonequilibrium of the freestream air and the ablation gas in the shock layer with an appropriate model for the finite-rate chemical reactions at the surface and the injection of the pyrolysis gas. In this paper, we present the analysis model for the viscous shock-layer flow with ablation injection in a framework of the nonequilibrium chemistry of the 19 carbon-oxygen-nitrogen species for ablation without the pyrolysis gas and the 26 carbon-oxygen-nitrogen-hydrogen species for ablation with the pyrolysis gas.

Under the severe wall heating condition, the surface of the ablator will become rough. The ablation gas injected to the boundary layer from such rough surface is expected to be turbulent. Park (1984) pointed out that the turbulence induced by the ablation injection may augment the convective heating rate not only in the downstream region but also in the stagnation region. We investigate the effects of the injection-induced turbulence on the convective heating rate over the forebody of the capsule by adapting Park's model to the VSL analysis.

The objectives of the present study are 1) to present the chemical nonequilibrium model of the shock layer flow with ablation injection and the boundary condition at the ablator surface, 2) to make the trajectory-based analysis on the aerodynamic heating environment for the MUSES-C superorbital re-entry capsule and 3) to assess the extent of the heating augmentation by the injection-induced turbulence.

2. METHOD OF ANALYSIS

2.1 Classification of Stagnation Flow Chemistry

Figure 1 shows the classification of the stagnation region flow chemistry for a sphere with the diameter 30.5 cm, which is close to that of the MUSES-C capsule, after Gupta et al. (1989). The effects of ablation are not considered. The number of the species to be considered in the analysis depends almost on the flight velocity, since the temperature behind the shock wave determines the chemical reactions to be excited. On the other hand, the extent of the chemical and thermal nonequilibrium effects depends on the flight altitude, since the rate of their equilibration depends on the air density. The flight trajectory of the MUSES-C capsule is also plotted in Fig. 1. It is clear that the 11-air-species, which consists of N\textsubscript{2}, O\textsubscript{2}, N, O, NO, NO\textsuperscript{+}, e\textsuperscript{−}, N\textsuperscript{+}, O\textsuperscript{+}, cies, which consists of N\textsubscript{2}, O\textsubscript{2}, N, O, NO, NO\textsuperscript{+}, e\textsuperscript{−}, N\textsuperscript{+}, O\textsuperscript{+}, N\textsubscript{2}\textsuperscript{+} and O\textsubscript{2}\textsuperscript{+}, and the chemical nonequilibrium of these species must be considered for the analysis in the flight regime of peak stagnation heating for the MUSES-C capsule. In addition to the 11-air-species (N\textsubscript{2}, O\textsubscript{2}, N, O, NO, O\textsuperscript{+}, e\textsuperscript{−}, N\textsuperscript{+}, O\textsuperscript{+}, N\textsubscript{2}\textsuperscript{+}, O\textsubscript{2}\textsuperscript{+}), we consider 8 carbon-nitrogen-oxygen species (C, C\textsubscript{2}, C\textsubscript{3}, CO\textsubscript{2}, CO, CN, CO\textsuperscript{+}, C\textsuperscript{+}) in relation to the gas injection at the ablator surface. Furthermore, the 7 carbon-nitrogen-oxygen-hydrogen species (H, H\textsubscript{2}, HCN, HO, C\textsubscript{2}H\textsubscript{2}, C\textsubscript{2}H, CH) are added to the above 19 species model when the effects of the surface injection of the pyrolysis gas of the ablator are considered.
2.2 Viscous Shock-Layer Analysis

The axi-symmetric viscous shock-layer (VSL) equations with chemical nonequilibrium and thermal equilibrium are solved by the finite difference method. The viscous shock-layer equations are obtained from the Navier-Stokes equations by retaining terms up to the second order in the Reynolds number parameter \( \varepsilon \) defined by:

\[
\varepsilon = \sqrt{\frac{\mu(T = u^2/\rho)}{\rho \cdot u \cdot \varepsilon}}
\]

where \( Rn \) is the nose radius. In the case of the MUSES-C capsule, the value of \( \varepsilon \) is in the order of \( 10^{-2} \) or \( 10^{-3} \) when the flight altitude is less than 75 km. Since our concern is mainly in the flight regime of the peak aerodynamic heating which occurs around 60 km altitude, the VSL analysis is expected to provide a sufficiently accurate solution of the shock layer over the blunt body with much smaller computation time in comparison with the Navier-Stokes analysis. The detail of the formulation is presented by Moss (1974). The non-dimensional VSL equations with the chemical nonequilibrium are given in a curvilinear, body-oriented coordinate system as follows:

**Global continuity equation:**

\[
\frac{\partial}{\partial s} [(r + y \cos \theta) \rho u] + \frac{\partial}{\partial y} [(1 + y \kappa) (r + y \cos \theta) \rho v] = 0
\]

**Streamwise momentum equation:**

\[
\rho \left( \frac{u}{1 + y \kappa} \right) \frac{\partial u}{\partial s} + \frac{\partial u}{\partial y} + \frac{w v k}{1 + y \kappa} + \frac{1}{1 + y \kappa} \frac{\partial p}{\partial s} = \varepsilon^2 \left\{ \mu \left( \frac{\partial u}{\partial y} - \frac{w v k}{1 + y \kappa} \right) + \mu \left( \frac{2 \kappa}{1 + y \kappa} + \frac{\cos \theta}{y + r \cos \theta} \right) \left( \frac{\partial u}{\partial y} - \frac{w v k}{1 + y \kappa} \right) \right\}
\]

Fig. 1: Classification of Stagnation Region Flow Chemistry.
Normal momentum equation:

\[ \rho \left( \frac{u}{1 + y\kappa} \frac{\partial v}{\partial s} + \frac{v}{1 + y\kappa} \frac{\partial u}{\partial y} - \frac{u^2\kappa}{1 + y\kappa} \right) + \frac{\partial p}{\partial y} = 0 \]  

Energy equation:

\[ \rho C_p \left( \frac{u}{1 + y\kappa} \frac{\partial T}{\partial s} + \frac{v}{1 + y\kappa} \frac{\partial T}{\partial y} \right) - \left( \frac{u}{1 + y\kappa} \frac{\partial p}{\partial s} + \frac{v}{1 + y\kappa} \frac{\partial p}{\partial y} \right) = \varepsilon^2 \left[ \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \left( \frac{\kappa}{1 + y\kappa} + \frac{\cos \theta}{r + y\cos \theta} \right) k \frac{\partial T}{\partial y} + \mu \left( \frac{\partial u}{\partial y} - \frac{u\kappa}{1 + y\kappa} \right)^2 - \sum_{i=1}^{N_s} J_i C_{pi} \frac{\partial T}{\partial y} \right] \]

Conservation equation of i-th species:

\[ \rho \left( \frac{u}{1 + y\kappa} \frac{\partial C_i}{\partial s} + \frac{v}{1 + y\kappa} \frac{\partial C_i}{\partial y} \right) = \dot{w}_i - \varepsilon^2 \frac{(1 + y\kappa) (r + y\cos \theta) J_i}{(1 + y\kappa) (r + y\cos \theta)} \left( \frac{\partial}{\partial y} \left[ (1 + y\kappa) (r + y\cos \theta) J_i \right] \right) \]  

In the above equations, \( s, y, r, \theta \) and \( \kappa \) are coordinate measured along the body surface, coordinate normal to the body surface, the radius measured from the axis of symmetry to a point on the body surface, the angle between the axis of symmetry and the body tangent, and the body curvature, respectively. \( u \) and \( v \) are the velocity components in \( s \) and \( y \) directions. \( C_i \) is the mass fraction of the \( i \)-th species. The diffusion mass flux of the \( i \)-th species \( J_i \) is considered only in the normal direction:

\[ J_i = -D_i \frac{\partial C_i}{\partial y}, \]

where the diffusion coefficient is given by using the Lewis number \( Le \) and the Prandtl number \( Pr \) as:

\[ D_i = D = Le \cdot \mu/Pr. \]  

The flow is assumed to be laminar except the case in the presence of the injection-induced turbulence. To simplify the finite-difference procedure, the VSL equations are transformed by normalizing the flow properties and the normal coordinate \( y \) with the flow properties behind the shock wave and the shock-layer thickness, respectively. The transformed equations and the method of solution are given by Moss (1974) and Miner et al. (1975).

For the stagnation heating environment analysis, only the stagnation streamline equations (Moss 1974) are solved. The downstream flow is solved by space marching technique efficiently with small computation time. For example, the computation time to obtain both the stagnation and the downstream solutions with 101 \( \times \) 41 grid points is less than 1 minutes on Fujitsu VPP-800 supercomputer at ISAS computer center. To keep the numerical stability of the space marching procedure, the coupling technique (Waskiewicz et al. 1978), where the normal momentum equation and the global continuity equation are solved in a coupled manner, is employed for the calculation of the pressure and the normal velocity component. The shock layer thickness is corrected after every streamwise sweep by considering the mass flux between the shock wave and the body surface. The convergence in the shock wave shape is obtained after five or six streamwise sweeps.
In the normal direction, the shock layer is divided into 101 grid points, which is clustered both to the wall and to the shock wave surface with the minimum spacing $3 \times 10^{-5}$ of the shock stand-off distance to obtain sufficient resolution of rapid change in the chemical composition there. In the VSL analysis, the computational domain is bounded by the shock wave surface and the body surface. The boundary conditions must be specified at both surfaces. The flow just behind the shock wave surface is assumed to be chemically frozen at the freestream composition and the boundary conditions are determined by the Rankine-Hugoniot relations. As for the boundary conditions at the capsule wall, we must consider the surface reactions of ablation. The chemistry model and the boundary condition at the ablator surface are explained in the following sections. Details of the present analysis model are also given by Suzuki et al. (1996; 1997; 1998).

### 2.3 Chemistry Model

The chemical reactions considered in the present analysis are listed in Table I. The reactions from No. 1 to 20 are related to the air species and their reaction rates are taken from Gupta’s 11-air-species model (Gupta et al. 1989). The reactions from No. 21 to 42 are related to the carbon-containing species and the reaction rates are taken from Blottner’s model (Blottner 1970) except the reactions 21, 22 and 23, which are from Song et al. (1986). The chemical reactions from No. 43 to 52 of the carbon-nitrogen-oxygen-hydrogen species (H, H₂, HCN, HCO, C₂H₂, C₂H, CH) are taken from Westbrook et al. (1984) except the reaction No. 44 (Heicklen 1967).

For the analysis of the superorbital re-entry, the air chemistry model must be valid up to 50000 K, since the maximum temperature behind the normal shock wave with frozen chemistry and thermal equilibrium exceeds 40000 K. For the thermodynamic properties of the 11 air species up to 30000 K, we use Gupta’s model (Gupta et al. 1989). For the air species at higher temperature and the 8 carbon-containing species, the thermodynamic properties are calculated by the partition function method (Allison 1966; Herzberg 1950). The thermodynamic properties of the carbon-nitrogen-oxygen-hydrogen species (H, H₂, HCN, HCO, C₂H₂, C₂H, CH) are taken from JANAF Thermochemical Tables (1985). For convenience in computation, the thermodynamic properties of each species are described by the polynomial curve-fit function of the temperature. The viscosity of each species is calculated by the curve-fit function of the temperature (Gupta et al. 1989; Blottner 1970). The thermal conductivity is obtained from the viscosity and the specific heat by Eucken’s empirical formula (Gupta et al. 1989). The viscosity and the thermal conductivity of gas mixture are calculated by Wilke’s method (Moss 1974). As seen in equations (7) and (8), the diffusion of the gas species is described by the binary diffusion model with the constant Lewis number of 1.4 (Moss 1974).

### 2.4 Boundary Condition at Ablator Surface

The schematic view of the chemical reaction model at the ablator surface is shown in Fig. 2. The mass fraction of the $i$-th species at the wall is determined by solving the surface mass balance equation written in the generalized form:

$$-\rho D_i \cdot (dC_i/dy) + \rho \cdot C_i \cdot v_{w} = J_i^{\text{out}} + J_i^{\text{ion}} + J_i^{\text{ox}} + J_i^{\text{sub}} + J_i^{\text{prop}}. \quad (9)$$

The first and the second terms of the left hand side represent the normal ($y$-direction) fluxes due to diffusion and ablation injection velocity $v_{w}$, respectively. In the present model,
Table 1: List of Chemical Reactions.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>No.</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$O_2 + M_1 \Leftrightarrow 2O + M_1$</td>
<td>27</td>
<td>$N_2 + C \Leftrightarrow CN + N$</td>
</tr>
<tr>
<td>2</td>
<td>$N_2 + M_2 \Leftrightarrow 2N + M_2$</td>
<td>28</td>
<td>$CO + N \Leftrightarrow CN + O$</td>
</tr>
<tr>
<td>3</td>
<td>$N_2 + N \Leftrightarrow 2N + N$</td>
<td>29</td>
<td>$CO_2 + N \Leftrightarrow CN + O_2$</td>
</tr>
<tr>
<td>4</td>
<td>$NO + M_3 \Leftrightarrow N + O + M_3$</td>
<td>30</td>
<td>$N_2 + CO \Leftrightarrow CN + NO$</td>
</tr>
<tr>
<td>5</td>
<td>$NO + O \Leftrightarrow O_2 + N$</td>
<td>31</td>
<td>$CO + NO \Leftrightarrow CO_2 + N$</td>
</tr>
<tr>
<td>6</td>
<td>$N_2 + O \Leftrightarrow NO + N$</td>
<td>32</td>
<td>$CO_2 + O \Leftrightarrow CO + O_2$</td>
</tr>
<tr>
<td>7</td>
<td>$N + O \Leftrightarrow NO^+ + e^-$</td>
<td>33</td>
<td>$2CO \Leftrightarrow CO_2 + C$</td>
</tr>
<tr>
<td>8</td>
<td>$O + e^- \Leftrightarrow O^+ + e^- + e^-$</td>
<td>34</td>
<td>$CO + O \Leftrightarrow O_2 + C$</td>
</tr>
<tr>
<td>9</td>
<td>$N + e^- \Leftrightarrow N^+ + e^- + e^-$</td>
<td>35</td>
<td>$CO + N \Leftrightarrow C + NO$</td>
</tr>
<tr>
<td>10</td>
<td>$O + O \Leftrightarrow O_2^+ + e^-$</td>
<td>36</td>
<td>$CN + O \Leftrightarrow C + NO$</td>
</tr>
<tr>
<td>11</td>
<td>$O + O_2^+ \Leftrightarrow O_2 + O^+$</td>
<td>37</td>
<td>$2CO \Leftrightarrow C_2 + O_2$</td>
</tr>
<tr>
<td>12</td>
<td>$N_2 + N^+ \Leftrightarrow N + N_2^+$</td>
<td>38</td>
<td>$CO + C \Leftrightarrow C_2 + O$</td>
</tr>
<tr>
<td>13</td>
<td>$N + N \Leftrightarrow N_2^+ + e^-$</td>
<td>39</td>
<td>$C_2 + CO \Leftrightarrow C_3 + O$</td>
</tr>
<tr>
<td>14</td>
<td>$O_2 + N_2 \Leftrightarrow NO + NO^+ + e^-$</td>
<td>40</td>
<td>$C_3 + C \Leftrightarrow 2C_2$</td>
</tr>
<tr>
<td>15</td>
<td>$NO + M_4 \Leftrightarrow NO^+ + e^- + M_4$</td>
<td>41</td>
<td>$C + O \Leftrightarrow CO^+ + e^-$</td>
</tr>
<tr>
<td>16</td>
<td>$O + NO^+ \Leftrightarrow NO + O^+$</td>
<td>42</td>
<td>$C + e^- \Leftrightarrow C^+ + e^- + e^-$</td>
</tr>
<tr>
<td>17</td>
<td>$N_2 + O^+ \Leftrightarrow O + N_2^+$</td>
<td>43</td>
<td>$H_2 + M_1 \Leftrightarrow 2H + M_1$</td>
</tr>
<tr>
<td>18</td>
<td>$N + NO^+ \Leftrightarrow NO + O^+$</td>
<td>44</td>
<td>$HCN + H \Leftrightarrow C_2N + H_2$</td>
</tr>
<tr>
<td>19</td>
<td>$O_2 + NO^+ \Leftrightarrow NO + O_2^+$</td>
<td>45</td>
<td>$HCO + M_2 \Leftrightarrow H + CO + M_{11}$</td>
</tr>
<tr>
<td>20</td>
<td>$O + NO^+ \Leftrightarrow O_2 + N^+$</td>
<td>46</td>
<td>$HCO + H \Leftrightarrow CO + H_2$</td>
</tr>
<tr>
<td>21</td>
<td>$CO_2 + M_5 \Leftrightarrow CO + O + M_5$</td>
<td>47</td>
<td>$C_2H_2 + M_3 \Leftrightarrow C_2H + H + M_{12}$</td>
</tr>
<tr>
<td>22</td>
<td>$CO + M_6 \Leftrightarrow C + O + M_6$</td>
<td>48</td>
<td>$C_2H_2 + H \Leftrightarrow C_2H + H_2$</td>
</tr>
<tr>
<td>23</td>
<td>$CO + O \Leftrightarrow C + O + O$</td>
<td>49</td>
<td>$C_2H_2 + O_2 \Leftrightarrow 2CHO$</td>
</tr>
<tr>
<td>24</td>
<td>$C_2 + M_7 \Leftrightarrow 2C + M_7$</td>
<td>50</td>
<td>$C_2H + O_2 \Leftrightarrow HCO + CO$</td>
</tr>
<tr>
<td>25</td>
<td>$C_3 + M_8 \Leftrightarrow C + C_2 + M_8$</td>
<td>51</td>
<td>$C_2H + O \Leftrightarrow CH + CO$</td>
</tr>
<tr>
<td>26</td>
<td>$CN + M_9 \Leftrightarrow C + N + M_9$</td>
<td>52</td>
<td>$CH + O_2 \Leftrightarrow HCO + O$</td>
</tr>
</tbody>
</table>

we consider four types of the surface reactions, that is, catalytic recombination of $N_2$ and $O_2$, recombination of ions and electron, surface oxidation and surface sublimation, and the injection of the pyrolysis gas as shown in Fig. 2. The surface mass balance equation for non-ablating wall is obtained by setting $J_{i}^{\text{cat}} = J_{i}^{\text{sub}} = J_{i}^{\text{pyro}} = 0$ in equation (9). The mass flux due to the catalytic recombination $J_{i}^{\text{cat}}$ is given by the finite catalytic wall (FiCW) model (Gupta et al. 1988):

$$J_{i}^{\text{cat}} = -\rho \cdot C_{i} \cdot \gamma_{i}^{\text{cat}} \sqrt{RT_{w}/2\pi M_{i}} \quad (i = N, O) \quad (10)$$
$$J_{i}^{\text{cat}} = -J_{i}^{\text{cat}}, \quad J_{O_2}^{\text{cat}} = -J_{O}^{\text{cat}}, \quad J_{i}^{\text{cat}} = 0 \quad (i = \text{others}), \quad (11)$$

where $T_{w}$ is the wall temperature, $M_{i}$ is the molecular weight and $\gamma_{i}^{\text{cat}}$ is the reaction probability for the catalytic recombination. The non-catalytic wall (NCW) and the fully catalytic wall (FCW) are described as $\gamma_{i}^{\text{cat}} = 0$ and $\gamma_{i}^{\text{cat}} = 1$, respectively. The mass flux due to recombination of ions and electron $J_{i}^{\text{ion}}$ is given in the same way. The thermochemical properties of the ablator surface is expected to be similar to those of graphite, since the surface of the carbon-
phenolic ablator becomes a char layer of solid carbon under the severe aerodynamic heating of superorbital reentry. Two types of reactions involving phase change at the surface, that is, oxidation by atomic oxygen and sublimation into C3 molecule, are considered. The mass flux due to the surface oxidation by atomic oxygen $J^{oxi}$ is presented after Blottner (1970):

$$J^{oxi} = -\rho \cdot C_i \cdot \gamma^{oxi} \frac{RT_w}{2\pi M_i}$$  \hspace{1cm} (i = O), \hspace{1cm} \text{(12)}$$

$$J^{oxi} = -J^{oxi}_O \cdot \frac{M_{CO}}{M_O}, \hspace{1cm} J^{oxi}_O = 0 \hspace{1cm} (i = \text{others}),$$  \hspace{1cm} \text{(13)}$$

where $\gamma^{oxi}$ is the reaction probability for oxidation of solid carbon by atomic oxygen. It should be noted that the constraint:

$$\gamma^{cat}_O + \gamma^{oxi}_O \leq 1$$  \hspace{1cm} \text{(14)}$$

exists, since the mass flux $-J^{cat}_O - J^{oxi}_O$ never exceeds the mass flux of atomic oxygen striking the wall. The surface mass flux due to sublimation is given by the Hertz-Knudsen-Langmuir relation (Blottner 1970):

$$J^{sub}_i = \alpha_i \cdot (p_{eq,i} - p_i) \sqrt{RT_w/2\pi M_i}$$  \hspace{1cm} (i = C_3), \hspace{1cm} \text{(15)}$$

$$J^{sub}_i = 0 \hspace{1cm} (i = \text{others}),$$  \hspace{1cm} \text{(16)}$$

where $p_{eq,i}$ and $p_i$ are the equilibrium vapor pressure and partial pressure of i-th species. We neglect sublimation into C and C2 gas, since the equilibrium vapor pressure for C3 gas is much higher than those species as shown in Fig. 3. The vaporization coefficient $\alpha_i$ for C3 molecule is set as 0.023.

The pyrolysis gas produced in the reaction zone of ablator interior is injected into the shock layer at the ablator surface and is expected to reduce the net heat flux to the surface. For the analysis including the pyrolysis gas, hydrocarbon species must be added to the chemistry model. In the present study, the pyrolysis gas is assumed to be composed of C3, CO, H2, C2H2 and C2H. To determine the injection rate of the pyrolysis gas and its composition, the Charring Material Ablator (CMA) analysis should be made by coupled procedure with the
aerodynamic heating environment analysis. In the present study, however, the pyrolysis rate and composition are specified beforehand. The case without pyrolysis, say, ablation of graphite, is described by setting $J_{\text{pyro}} = 0$.

The ablation injection velocity at the wall $v_w$ is determined by the surface mass loss rate $m_w$ and the pyrolysis rate $m_p$:

$$m_w + m_p = J_{\text{sub}}^C - J_{\text{sub}}^{CO} \cdot (M_C/M_O) + \sum_{r=\text{pyro}} J_{\text{pyro}}^r = \rho_w \cdot v_w \quad (17)$$

To obtain the gas composition and the ablation injection velocity at the surface, the equations (9) and (17) must be solved simultaneously by an iterative procedure.

The net convective heating rate to the ablator surface is defined by considering the energy transport by ablation injection as:

$$\dot{q}_{c,\text{net}} = k(\partial T/\partial y)_w + \sum_t (h_t \cdot \rho C_t \cdot (\partial C_t/\partial y)_w)$$
$$- [(m_w + m_p)h_w - (J_{\text{sub}}^C h_{CO} + J_{\text{sub}}^{CO} h_{O}) - J_{\text{sub}}^C h_{C_2} - m_p h_{pyro}] \quad (18)$$

The wall temperature is predicted by neglecting the heat flux transported into the ablator interior and considering the energy balance at the surface including the heat of phase change at ablator surface and radiative cooling as:

$$\dot{q}_{c,\text{net}} = (m_{\text{oxi}} \Delta h_{\text{oxi}} + m_{\text{sub}} \Delta h_{\text{sub}}) + \varepsilon \sigma \cdot T_w^4, \quad (19)$$

where the ablator surface emissivity $\varepsilon$ is set as 0.725 (Ahn et al. 1997).

2.5 Injection-Induced Turbulence Model

To assess the extent of the convective heating augmentation due to the turbulent gas injection from rough ablator surface, the injection-induced turbulence model by Park (1984) is adapted.
to the VSL analysis. In the turbulent VSL analysis, the molecular viscosity $\mu$ is replaced by the effective viscosity $\mu_{eff} = \mu + \mu_t$, where $\mu_t$ is the eddy viscosity. The eddy viscosity is described by using turbulence energy $\varepsilon$ and the mixing length $d$:

$$\mu_t = \frac{1}{\varepsilon^2} \cdot C_\mu \cdot \rho \cdot \sqrt{\varepsilon} \cdot d,$$

where $\varepsilon$ is the Reynolds number parameter defined in equation (1). The governing equation of the turbulence energy is given in the standard VSL notation (Moss 1974):

$$\rho \cdot \left\{ \frac{u}{1 + n\kappa} \cdot \frac{\partial e}{\partial s} + v \cdot \frac{\partial e}{\partial n} \right\} = \varepsilon^2 \left[ \frac{\partial}{\partial n} \left( \frac{\mu_{eff}}{P_{eff}} \right) \frac{\partial e}{\partial n} \right] + \left( \frac{\kappa}{1 + n\kappa} + \frac{\cos \theta}{r + n \cos \theta} \right) \cdot \left( \frac{\mu_{eff}}{P_{eff}} \right) \frac{\partial e}{\partial n}$$

$$+ \varepsilon^2 \mu_t \cdot \left( \frac{\partial u}{\partial n} - \frac{\kappa u}{1 + n\kappa} \right)^2 - \frac{C_D \cdot \rho \cdot \varepsilon^{3/2}}{d}.$$

The mixing length $d$ is assumed to be in the same order as the surface roughness scale and to be constant through the shock layer. The eddy viscosity at the ablating wall is given by:

$$\mu_{t,w} = K \cdot \rho_w \cdot v_w \cdot d,$$

where $K$ is the von Kármán constant. From equations (20) and (22), the turbulence energy at the wall is given as:

$$\varepsilon_w = \left( \frac{K}{C_\mu} \cdot v_w \right)^2.$$

The constant $C_\mu, C_D, K$ are set as 0.22, 0.42, 0.4, respectively. The turbulent thermal conductivity and diffusion coefficient are calculated by assuming the turbulent Prandtl number 0.9 and the turbulent Lewis number 1.0 (Moss 1981).

### 3. RESULTS AND DISCUSSION

#### 3.1 Capsule Configuration and Re-entry Trajectory

Figure 4 shows the nominal reentry trajectory of the MUSES-C sample-return capsule. The horizontal axis represents the time from the flight altitude at 200 km. The temporal variations of the stagnation convective and radiative heating rates predicted by Tauber's empirical formulas (Tauber et al. 1990; 1991) are also plotted in the figure. The peak stagnation convective heating is expected to occur at the flight velocity around 11.6 km/s and flight altitude around 64 km. The computation has been done at the flight conditions listed in Table 2. The MUSES-C capsule has an axi-symmetric blunt cone configuration with nose radius $Rn$ of 0.2 m, semiapex angle of 45 deg and base diameter of 0.4 m. Figure 5 shows the capsule configuration and the definition of the computational coordinates. The reaction probability of the surface oxidation of the ablator is set as unity ($\gamma_{oxi} = 1$). We assume that the ablating wall is non-catalytic, since the significant catalytic recombination has not been observed in the heating experiments of graphite (Park 1976; Ahn et al. 1997). The surface injection of the pyrolysis gas is not considered except the cases of Section 3.5.
3.2 VSL Analysis without Ablation

Figure 6 shows the temporal variations of the stagnation convective heating along the trajectory of the MUSES-C capsule. Both the 11-air-species model \((\text{N}_2, \text{O}_2, \text{N}, \text{O}, \text{NO}, \text{NO}^+, \text{e}^-, \text{N}^+, \text{O}^+, \text{N}_2^+ \text{ and } \text{O}_2^+)\) and the 7-air-species model \((\text{N}_2, \text{O}_2, \text{N}, \text{O}, \text{NO}, \text{NO}^+ \text{ and } \text{e}^-)\) are considered. Ablation is not considered. Two limiting cases with respect to the wall catalycity, that is, the non-catalytic wall (NCW) and the fully catalytic wall (FCW) are calculated. At NCW, no chemical reactions occur at the wall and the normal gradient of the mass fraction of each species vanishes there. At FCW, the chemical composition at the wall is assumed to become the same as that of the freestream air due to the catalytic recombination reactions. The wall
Table 2: Calculation Conditions along Re-entry Trajectory of MUSES-C Capsule.

<table>
<thead>
<tr>
<th>Case</th>
<th>Time from 200 km altitude (s)</th>
<th>Velocity (km/s)</th>
<th>Altitude (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>80.0</td>
<td>12.4</td>
<td>72.1</td>
</tr>
<tr>
<td>2</td>
<td>85.0</td>
<td>12.1</td>
<td>67.8</td>
</tr>
<tr>
<td>3</td>
<td>90.0</td>
<td>11.6</td>
<td>64.0</td>
</tr>
<tr>
<td>4</td>
<td>95.0</td>
<td>10.9</td>
<td>60.7</td>
</tr>
<tr>
<td>5</td>
<td>100.0</td>
<td>9.91</td>
<td>57.9</td>
</tr>
<tr>
<td>6</td>
<td>105.0</td>
<td>8.79</td>
<td>55.5</td>
</tr>
<tr>
<td>7</td>
<td>110.0</td>
<td>7.62</td>
<td>53.5</td>
</tr>
<tr>
<td>8</td>
<td>120.0</td>
<td>5.49</td>
<td>50.2</td>
</tr>
<tr>
<td>9</td>
<td>130.0</td>
<td>3.88</td>
<td>47.6</td>
</tr>
</tbody>
</table>

temperature is assumed to be constant at 1200 K. The results show that the 7-air-species model provides higher heating rate than the 11-air-species model both for the NCW case and for the FCW case. However, after $t = 110$ sec, i.e. at flight velocity lower than 8 km/s, their difference becomes negligibly small. Figure 7 shows the temperature distributions on the stagnation streamline at $t = 90$ sec (Case 3 in Table 2) and $t = 110$ sec (Case 7 in Table 2). The temperature rapidly decreases behind the shock wave due to dissociation of molecular species and reaches the plateau in the middle of the shock layer. At $t = 110$ sec, the difference between two models is hardly observed as already seen in the stagnation heating rate (see Fig. 6). At $t = 90$ sec, the plateau in the temperature distribution by the 7-species model is much higher than that by the 11-species model by about 5000 K. The reason for this discrepancy is that the ionization of N and O by electron impact which is not included in the 7-species model:

$$N + e^- \rightarrow N^+ + e^- + e^-,$$
$$O + e^- \rightarrow O^+ + e^- + e^-$$

becomes significant at velocity higher than 8 km/s and that the 7-species model underpredicts the rate of ionization. Consequently, the 11-species model must be considered at velocity higher than 8 km. The wall heating rate is significantly augmented due to the wall catalycity through the flight regime shown in Fig. 6. This fact indicates that the shock-layer flow is still in chemical nonequilibrium even when the flight altitude reaches 50 km. The prediction by the empirical relations (Tauber et al. 1990; 1991) is also plotted in Fig. 6. Both in the VSL analysis and in the empirical prediction, the maximum convective heating occurs at time between 90 sec and 100 sec. The heating rate by the empirical prediction is very close to the VSL analysis with the FCW assumption, which indicates the upper limit of the wall heating augmentation due to the wall catalycity.

3.3 Stagnation Heating Environment with Ablation

Figure 8 shows the variation of the surface mass loss rate with the wall temperature at Case 3. Both the diffusion-controlled regime and the sublimation regime are successfully described by the present model. When the wall temperature is between 1500 K and 3000 K, the surface mass loss is in the diffusion-controlled regime and its rate is hardly affected by the wall temperature,
since the surface mass loss is dominated by the oxidation of solid carbon and the extent of this reaction is limited by the capability of the transport of the atomic oxygen to the wall by the diffusion. When the wall temperature exceeds 3000 K, sublimation of solid carbon becomes significant and the mass loss rate rapidly increases with the wall temperature. Note that the rate-controlled regime of the surface mass loss is not described in the present model, since the reaction probability of the surface oxidation is assumed to be constant. The surface mass loss rate predicted by the present analysis is higher than that by Metzger’s semiempirical relation (Metzger 1967) (shown as dashed line in the figure). There are two possible reasons. One is the effect of the nonequilibrium chemistry. Metzger’s relation is based on the experimental
data obtained in dense arc-heated flow environment, where the shock layer flow is expected to be near the equilibrium state. The other reason is the inaccuracy in the analysis model. If so, that may be mainly attributed to the diffusion model, since in the diffusion-controlled regime, the surface mass loss rate is sensitive to the diffusion flux of atomic oxygen and less sensitive to the reaction probability of the surface oxidation. We use the simple model of the constant Lewis number 1.4 for the diffusion transport. For accurate prediction of the surface mass loss rate, more sophisticated model may be necessary for the diffusion transport.

Figure 9 shows the temporal variation of the stagnation-point wall temperature along the re-entry trajectory for the cases of the fully-catalytic wall (FCW) without ablation, no surface reactions and the ablating wall. The wall temperature with ablation is much reduced in comparison with the FCW case. After time 100 sec, however, the temperature of ablating wall becomes higher than that of the non-reacting wall, since the wall temperature still remains in the diffusion-controlled regime, and the surface oxidation reaction results in heat release to the surface. When the surface injection of the pyrolysis gas is considered for the ablating case, the wall temperature is expected to be significantly reduced as discussed later. The temporal variation of the surface mass loss rate is shown in Fig. 10. After the peak wall temperature at time 100 sec in Fig. 9, the surface mass loss rate decreases quite slowly because it is not sensitive to the wall temperature in the diffusion-controlled regime, as shown in Fig. 8.

![Graph showing the variation of surface mass loss rate with wall temperature.](image)

Fig. 8: Variation of Surface Mass Loss Rate with Wall Temperature.

### 3.4 Heating Environment in Downstream Region

Figure 11 shows the streamwise distributions of the net convective wall heating rate in Case 3 for the non-ablating wall at temperature 3000 K, ablating wall at 3000 K and ablating wall at 3600 K. The non-catalytic and iso-thermal wall is assumed. When the wall temperature is 3000 K and the ablation process is in the diffusion-controlled regime, slight reduction in the net convective heating due to ablation is observed only in the stagnation region. On the other hand, when the wall temperature is 3600 K, the ablation process is in the sublimation regime.
and the net convective heating is significantly reduced by ablation both in the stagnation region and in the downstream region.

Figure 12 shows the distributions of the surface mass loss rate and the ablation injection velocity along the body. In the diffusion-controlled regime ($T_w=3000$ K), the injection velocity is almost constant, since the reaction speed of oxidation depends on the square root of the wall temperature (see equation (12)) and we assume the iso-thermal wall. In the sublimation regime ($T_w=3600$ K), however, the sublimation at the surface becomes significant and the mass flux of surface mass loss consists of the oxidation part and the sublimation part. The difference
between the mass loss rate at the wall temperature 3600 K and that at 3000 K is expected to represent the extent of sublimation. It seems almost constant over the surface, since the mass flux of sublimation depends on the equilibrium vapor pressure which is determined by the wall temperature. Consequently, in the sublimation regime, the injection velocity may increase in the downstream direction, since the mass flux of sublimation is almost constant over the surface and the gas density at the wall decreases in the downstream direction as well as the wall pressure. In fact, the peak injection velocity is observed not at the stagnation point but at the junction between the spherical part and the conical part (s/Rn=0.8 in the figure) in the case of the wall temperature 3600 K.

![Distribution of Net Convective Heating Rate along the Surface with and without Ablation.](image)

**Fig. 11:** Distribution of Net Convective Heating Rate along the Surface with and without Ablation.

### 3.5 Effects of Pyrolysis Gas Injection

The injection of pyrolysis gas is expected to reduce the convective heating. To evaluate the blocking efficiency of the ablation injection, the blowing parameter $B$:

$$ B = \frac{(\dot{m}_w + \dot{m}_p) \cdot C_{P\infty}(T_B - T_w)}{q_{cold}} $$

and the blocking efficiency are introduced. The blocking efficiency is defined as the ratio of the net convective heating rate with ablation to the heating rate without ablation, that is, the cold wall heat flux $q_{cold}$. We consider three types of the pyrolysis composition specified by the mass fractions as:

- **Pyro - 1**: CO$_2$ 100%
- **Pyro - 2**: CO : H$_2$ = 0.93 : 0.07
- **Pyro - 3**: CO : C$_2$H : C$_2$H$_2$ : C$_3$ : H$_2$ = 0.35 : 0.35 : 0.15 : 0.10 : 0.05

*Pyro - 3* is an approximation to the chemical equilibrium composition of the pyrolysis gas of phenolic resin at 3600 K. The pyrolysis rate is assumed to be constant at 0.005 g/cm$^2$/sec, which
is in the same order as the surface mass loss rate. The relation between the blowing parameter and the blocking efficiency at the stagnation point in Case 3 is shown in Fig 13. The variation of the blowing parameter is obtained by changing the wall temperature from 2000 K to 3600 K. The dashed line in the figure indicates the empirical relation by Marvin (1967). Results show that reduction in the net convective heating by ablation with pyrolysis of hydrocarbon is greater than that by ablation without pyrolysis and that the blocking effect depends on the composition of pyrolysis gas.

Figure 14 shows the distributions of the mass fractions of CO and hydrocarbon species on the stagnation streamline for Pyro – 3 case. The wall temperature is 3000 K. The pyrolysis gas of C2H, C2H2, H2 is rapidly dissociated into H and CH. Such dissociation reactions are expected to enhance the blocking effect by heat absorption.

3.6 Effects of Injection-Induced Turbulence

Figure 15 shows the variation of the blocking efficiency at the stagnation point with the blowing parameter for the laminar and turbulent injection in Case 3. The mixing length of the turbulence is assumed to be constant as 2 mm. The augmentation of the peak stagnation-point convective heating rate due to the injection-induced turbulence is expected to be negligibly small, since the freestream Reynolds number based on the nose radius is in the order of 10^4 in the flight regime of the peak aerodynamic heating and is not enough to make the eddy viscosity significant even when the surface roughness is as large as 1 mm.

However, the turbulence energy of the ablation injection may be augmented in the downstream region. Figure 16 shows the streamwise distribution of the net convective heating rate in Case 3. The non-catalytic and iso-thermal wall at 3000 K is assumed. The mixing length for the turbulent analysis is 0.5 mm. It is observed that the peak heating for the turbulent case occurs in the downstream region of the stagnation point because of the production term in the turbulent energy equation (21) (the last term in the right hand side). Consequently, care must be taken for the presence of the peak heating due to the injection-induced turbulence in the downstream region.
4. CONCLUDING REMARKS

The ablation phenomena are formulated in a framework of the nonequilibrium chemistry of the 26 carbon-oxygen-nitrogen-hydrogen species. The boundary conditions at the ablator surface are presented by considering the reactions at the surface of solid carbon and the injection of the pyrolysis gas. The major conclusions obtained by the VSL analysis for the MUSES-C superorbital re-entry capsule are as follows:
(1) Both the diffusion-controlled regime and sublimation regime in the mass loss process at the ablator surface are successfully described by the present model.

(2) The stagnation wall temperature with ablation becomes much lower than that of the fully-catalytic non-ablating wall. Due to heat release of the surface oxidation reaction, however, the temperature of the ablating wall is higher than that of non-reacting wall.
(3) The net convective wall heating rate is significantly reduced by the surface injection of the pyrolysis gas of hydrocarbon.

(4) In the range of the freestream Reynolds number of the flight trajectory of the MUSES-C capsule, the augmentation of the convective heating due to the injection-induced turbulence is negligibly small at the stagnation point. In the downstream region, however, the turbulence energy is augmented and the peak heating may occur in the downstream of the stagnation point.

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A Thermochemical Nonequilibrium Flow around a Super Orbital Reentry Capsule with Ablation

By

Ryouji DOIHARA; and Michio NISHIDA†

(1 February 2003)

Abstract: The aerodynamic heating to the super orbital reentry capsule of MUSES-C with ablation was numerically studied by using thermochemical nonequilibrium full viscous shock layer (VSL) equations. An 11 air-species model was used for non-ablating boundary conditions, and six carbonic species were added for ablating boundary conditions. With a three-temperature model, thermal nonequilibrium effect was taken into account. The convective and radiative heat fluxes to the wall were examined for both fully catalytic wall (FCW) condition and non-catalytic wall (NCW) condition at various altitudes for the capsule reentry trajectory path. The results of the ablation analysis at the altitude of 64 km showed that the stagnation heat fluxes with and without ablation are almost equal below the wall temperature of 3,000 K, whereas at the wall temperatures over 3,000 K, the stagnation heat flux is rapidly decreased with an increase in wall temperature due to significant sublimation.

1. INTRODUCTION

In the MUSES-C project the capsule is to enter into the earth’s atmosphere directly from the hyperbolic earth-return trajectory. Therefore, 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.

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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 (Sakamura & Nishida 1991, Gupta 1996, Suzuki et al. 1996, Doihara & Nishida 2002). Of these, Suzuki et al. (1996) is cited as the work treating a super-orbital reentry. In their work, the flowfield over the MUSES-C capsule was analyzed using a two-temperature model consisting translational-rotational and vibrational-electron temperatures, and aerodynamic heating to the capsule for both 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 thermal nonequilibrium should be calculated more accurately. The MUSES-C capsule will have a heat shield made of C/C composite material. The carbonic 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 carbonic 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 with ablation. 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 carbonic 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 & Abe (1997).

2. METHOD OF ANALYSIS

2.1 Governing Equations

The governing equations are the full viscous shock layer (FVSL) 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. These equations are written for an axisymmetric body-intrinsic coordinate system \((s,y)\) as shown in Fig. 1. 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. In the full viscous shock layer (FVSL) analysis, the second order \( y \)-momentum equation is used.

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. (Fig. 1).

The following assumptions are introduced:

1) Rotational temperature of molecules is fully equilibrated with translational temperature of heavy particle.
2) Translational-rotational temperatures of all the species are equal.
3) Vibrational temperatures of all the molecular species are equal.
4) Electronic temperatures of N, N⁺, O, O⁺, O₂ are equal and fully equilibrated with electron temperature.

5) Emission and absorption of radiation are not considered in the VSL calculation. Radiative heat flux is estimated from the results of the VSL analysis.

The present governing equations are composed of tangential momentum, normal momentum, translational-rotational energy, vibrational energy, electron-electronic energy and species conservation equations. They are written in fashion similar to Miner & Lewis (1975).

2.2 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 (Gupta et al. 1990). For ablation analysis, the viscosity and thermal conductivity for a mixture of gas have been computed using the Wilke's semi-empirical formula and Yos' formula. Viscosity of each species can be determined from the curve fit form of Blottner (1970) and the curve fit data for the species can be taken from Olynick et al. (1999). The diffusion coefficients of Curtiss & Hirschfelder (1949) are used. For ions, ambipolar diffusion is assumed.

2.3 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 & White (1963) and the correction term of Park's collision limit (Park 1993). The translation-electron and rotation-electron energy transfer rates are taken from Lee (1985), and Lazdins & Petrie (1974), 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 (1992). The average vibrational energy removed by dissociation is assumed to be 50 % of dissociation energy.

2.4 Air chemistry

In 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 % N₂ + 23.5 % O₂ in the
freestream) model consisting of \( N_2, O_2, NO, N, O, NO^+, O^+, N^+, N_2^+, O_2^+ \) and \( e^- \). We consider reactions of these 11 species given in Table 1. The chemical reaction rate model is the Park model (Park 1993) that uses effective temperature extended to a three temperature model. Reaction rates are assumed to be a function of controlling temperatures \( T_f \) and \( T_b \) depending on the type of reaction, and they are given by the following expressions:

\[
k_{f,r}(T_{f,r}) = C_r T_{f,r}^s \exp(-\theta_r/T_{f,r}) \tag{1}
\]

\[
k_{b,r}(T_{b,r}) = k_{f,r}(T_{b,r})/K_r^{eq}(T_{b,r}) \tag{2}
\]

where \( K_r^{eq}(T_{b,r}) \) is the equilibrium constant. The controlling temperatures are shown in Table 1. The values of \( C_r \), \( s_r \) and \( \theta_r \) can be obtained from Park (1993).

For the ablation analysis, the 19 chemical reactions of 6 carbon-containing species are added to the 11 air species. The reaction rates of the 19 reactions are taken from Blottner (1970) and shown in Table 2.

<table>
<thead>
<tr>
<th>( r )</th>
<th>Reactants</th>
<th>Products</th>
<th>( T_f )</th>
<th>( T_b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( N_2 + M_1^p )</td>
<td>( N + N + M_1 )</td>
<td>( \sqrt{T \cdot T_{vib}} )</td>
<td>( T )</td>
</tr>
<tr>
<td>2</td>
<td>( N_2 + M_2^p )</td>
<td>( N + N + M_2 )</td>
<td>( \sqrt{T \cdot T_{vib}} )</td>
<td>( T )</td>
</tr>
<tr>
<td>3</td>
<td>( N_2 + e^- )</td>
<td>( N + N + e^- )</td>
<td>( \sqrt{T_a \cdot T_{vib}} )</td>
<td>( \sqrt{T \cdot T_a} )</td>
</tr>
<tr>
<td>4</td>
<td>( O_2 + M_1 )</td>
<td>( O + O + M_1 )</td>
<td>( \sqrt{T \cdot T_{vib}} )</td>
<td>( T )</td>
</tr>
<tr>
<td>5</td>
<td>( O_2 + M_2 )</td>
<td>( O + O + M_2 )</td>
<td>( \sqrt{T \cdot T_{vib}} )</td>
<td>( T )</td>
</tr>
<tr>
<td>6</td>
<td>( NO + M_3^p )</td>
<td>( N + O + M_3 )</td>
<td>( \sqrt{T \cdot T_{vib}} )</td>
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</tr>
<tr>
<td>7</td>
<td>( NO + M_4^p )</td>
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<td>( \sqrt{T \cdot T_{vib}} )</td>
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</tr>
<tr>
<td>8</td>
<td>( N_2 + O )</td>
<td>( NO + N )</td>
<td>( T )</td>
<td>( al )</td>
</tr>
<tr>
<td>9</td>
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<td>( NO + N )</td>
<td>( T )</td>
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<tr>
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<td>( N_2^+ + e^- )</td>
<td>( T )</td>
<td>( T )</td>
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<td>( T )</td>
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<td>( T )</td>
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<td>( T )</td>
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<tr>
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<td>( T )</td>
<td>( T )</td>
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<td>( T )</td>
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</tr>
<tr>
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<td>( N_2^+ + O )</td>
<td>( T )</td>
<td>( T )</td>
</tr>
<tr>
<td>23</td>
<td>( N + e^- )</td>
<td>( N^+ + e^- + e^- )</td>
<td>( T_a )</td>
<td>( T_e )</td>
</tr>
<tr>
<td>24</td>
<td>( O + e^- )</td>
<td>( O^+ + e^- + e^- )</td>
<td>( T_e )</td>
<td>( T_e )</td>
</tr>
</tbody>
</table>

\(^a M_1 = N_2, O_2, NO, N_2^+, O_2^+, NO^+ \)
\(^b M_2 = N, O, N^+, O^+ \)
\(^c M_3 = N_2, O_2, N_2^+, O_2^+ \)
\(^d M_4 = NO, N, O, NO^+, N^+, O^+ \)

2.5 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 Miner & Lewis (1975). These equations are rewritten in a tridiagonal matrix by using a second order finite difference method. The tridiagonal matrix is easily solved using the 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 \( \frac{W^{k+1} - W^k}{\Delta} \) is added to the standard parabolic form:

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

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 \( C_i \). 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.

2.6 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 \((\partial C_i/\partial y)_w = 0\) or fully catalytic wall (FCW) condition \(C_i = C_{i,\infty}\), where \(C_i\) is the mass concentration of species \(i\). The wall temperature \(T_w\) is assumed to be constant at 2,500 K in the non-ablation analysis. The vibrational temperature on the wall is also assumed to be equal to the wall temperature. The boundary condition of the electron temperature is calculated by Eq.(10) in Nishida (1972) that is derived from the Langmuir probe theory. Boundary conditions immediately behind the shock are determined by shock jump conditions from free stream conditions on the reentry trajectory (Fig. 2). To consider low density gas effect, shock boundary conditions are determined by using shock slip conditions (Miner & Lewis 1975). 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

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

where

\[
K_{w,\text{oxi}} = \alpha \sqrt{\frac{RT_w}{2\pi M_O}}
\]
and $M_{CO}$ and $M_O$ are, respectively, the molecular weights of CO and O. The reaction probability $\alpha$ is given as follows (Park 1976):

$$\alpha = 0.63 \exp\left(-11601/T^*\right)$$

(6)

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 (Blottner 1970):

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

(7)

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 $P_{e, C_3}$ were given in Blottner (1970).

2.7 Radiation Calculation

The VSL analysis is not coupled with the calculation of radiative heat transfer. Radiation analysis is performed by SPRADIAN (Fujita & Abe 1997) in non coupled manner, using flow field on the stagnation stream line calculated by the VSL code. In the estimation of radiative heat flux, the spherical cap model (Fujita & Abe 1997) is used for the integration of the heat transfer equation.

3. RESULTS AND DISCUSSION

The non-ablation analysis revealed that the heat fluxes for FCW and NCW have the maximum of 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 transfer becomes significant at the altitudes from 70 km to 55 km. At these altitudes, so called avalanche ionization phenomenon (Park 1990) leads to larger electron density and temperature, and as a result radiative heating becomes strong. The maximum radiative heating is approximately 0.9 MW/m$^2$ at the altitude of 62 km. The difference between the radiative heat fluxes for NCW and FCW cannot be seen. On the other hand,

Figures 3 and 4 illustrate the results of the ablation analysis, that is the distribution of the mole fractions on the stagnation streamline ($H=64$ km, $T_w=2,500$ K, 19 species model). In all the ablation analyses, the air species are assumed to be fully catalytic on the wall. 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 ($N + e^- \rightarrow N^+ + e^- + e^-$). 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 (Park 1990). At this wall temperature ($T_w=2,500$ 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 carbonic species on the stagnation streamline in case of $T_w = 3,200$ K. It is seen that the mol fraction of $C_3$ is comparatively large in the vicinity of the wall, that means significant sublimation of $C_3$. In the region away from the wall, $C_3$ is
rapidly dissociated into \( \text{C}_2 \) and \( \text{C} \), and then these two species and air species recombined into \( \text{CN} \) and \( \text{CO}_2 \).

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 \( T_w = 2,500 \text{ K} \), the stagnation heat fluxes with and without ablation are almost equal. At the wall temperatures above 3,000 K, where the sublimation becomes significant, the stagnation heat flux with ablation is rapidly reduced.

Figure 7 illustrates radiation spectra with and without ablation that was calculated by SPRADIAN (Fujita & Abe 1997) on the stagnation point at the altitude of 64 km \( (T_w=3,200 \text{ K}) \). The strong emission line spectra from \( \text{N} \), \( \text{N}^+ \) and \( \text{O} \) are identified below 2,000 Å and over 7,000 Å.
Fig. 7: Radiation density at the stagnation point with ablation ($H = 64$ km, $T_w = 3,200$ K).

Å. $N_2^+$ (1-) 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 $C_2$(Swan) are observed. The radiative heat flux with ablation is 0.96 MW/m².

4. CONCLUDING REMARKS

Aerodynamic heating to the super orbital reentry capsule has been numerically analyzed by using the full viscous shock layer equations with a three temperature model and nonequilibrium air chemistry.

It has been found from the non-ablation analysis 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, 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 for both NCW and FCW.

The ablation by the sublimation becomes significant at the wall temperature higher than 3,000 K and reduces the wall heat flux largely. On the other hand, when the wall temperature is low, the ablation occurs only by the oxidation, which leads to the fact that the wall heat flux is hardly reduced by the ablation due to oxidation. The ablation species slightly increase the radiative heat flux.
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Influences of Transport Model on Heating Rate of Reentry Vehicles

By
Hirotaka Otsu, Kazuhisa Fujita, and Takashi Abe

(1 February 2003)

Abstract: We assessed the effect of the models of transport properties for the estimation of the hypersonic reentry heating environment from an engineering point of view. Among the transport properties, we focus on the diffusion of chemical species. For this purpose, the following three models: Stefan-Maxwell model, Yos model, and Lee model are evaluated. The nominal flight condition for the evaluation is the reentry speed of 11.6 km/s at the altitude of 64 km, which corresponds to the most severe reentry flight condition for a super-orbital reentry such as MUSES-C mission. In the nominal flight condition case, under both the non-catalytic wall condition and the full-catalytic wall condition, the Lee model shows a discrepancy with the other two models and gives a higher heat flux. On the contrary, the Stefan-Maxwell model and the Yos model show a reasonably good agreement between them. The discrepancy between the Lee model and the others is caused by the contribution of diffusion of enthalpy. The discrepancy between the Lee model and the others increases with an increase of the flight velocity while the discrepancy shows only a negligible dependency on the atmospheric density. The increase of the discrepancy is attributed to the increase of the chemical species of dissociated air with the increase of the flight velocity. Because of this, even the Lee model is acceptable in a low reentry speed range such as a reentry from LEO. However the Lee model is hardly acceptable for an application to the higher velocity reentry such as a super-orbital reentry. On the other hand, the discrepancy between the Stefan-Maxwell model and the Yos model is reasonably small in all the circumstance. As for the calculation cost, the Stefan-Maxwell model is about two times expensive than other two models. Therefore, in a view point of estimating the heat flux for the hypersonic reentry flight vehicle with a reasonably accuracy and a reasonably computation cost, the Yos model is the most recommendable among the three models considered in this study.

1. Introduction

One of the key technologies for reentry missions is the development of the thermal protection system (TPS) for the reentry vehicle. For the design of TPS, the estimation of the heat flux to the reentry vehicle is a most critical subject. Among the heat flux to the reentry vehicle, which comprises of the convective and radiative parts, we will focus on the convective heat flux.
in this study. This is because the radiative heat flux is smaller than the convective heat flux even in a hyperbolic reentry which is required for MUSES-C mission (Kawaguchi et al. 1996) and, therefore, the convective heat flux was of primary interest for the reentry vehicle.

For the estimation of the convective heat flux in the real flight condition, the ground experimental facility cannot attain the real flight condition. Hence the computational fluid dynamics (CFD) technique is an alternative and promising method for the estimation of the convective heat flux. Needless to say, in order to obtain a reliable result from the CFD calculation, a suitable selection of the flow model, such as chemical reactions, thermal non-equilibrium and transport phenomena, is very important for an accurate estimation of the aerodynamic heating. This is because the flow model has a strong influence on the prediction of the flow field.

In the MUSES-C mission, the flow around the capsule is predicted to be thermally and chemically nonequilibrium at the altitude where the aerodynamic heating reaches its maximum value. In such a flow, the convective heat flux is composed of three terms; the conduction of energy due to the gradient of translational-rotational temperature, $T$, the conduction of energy due to the gradient of vibrational-electronic temperature, $T_V$, and the diffusion of enthalpy due to the concentration gradients of each chemical species. In the boundary layer, both temperatures are expected to be almost in equilibrium. Thus, the thermal conductivity inherent to them reflects an amount of the heat flux arising from their gradient at the boundary. The third term is related to the diffusion. All the three components are expected to be strongly dependent on the transport properties such the heat conductivity and the diffusion coefficients. This means that the models for the transport properties must be accurate and the accuracy of the models for the transport coefficients will have a large impact on the estimation of the convective heat flux to the reentry vehicle. Hence we must pay much attention to the selection of the models of transport properties for estimation of the convective heat flux. Among the transport properties, the model for the heat conductivity widely accepted (Gnoffo et al. 1989) is comparably reliable while there are several models for the diffusion coefficients. In this study, we evaluate numerically the widely-used models for the diffusion coefficient in a viewpoint of both the accuracy in estimation of the reentry heating environment under the various reentry flight conditions and the computational cost.

2. Aerothermal models

In this study, we consider an aerodynamic heating environment for the super-orbital reentry such as the MUSES-C mission (Kawaguchi et al. 1996; Otsu et al. 1998). To assess numerically the aerodynamic heating environment, the following governing equation for the thermally and chemically nonequilibrium flow (Gnoffo et al. 1989) is employed:

$$\frac{\partial U}{\partial t} + \frac{\partial F_j}{\partial x_j} = S,$$

where $U$, $F_j$, and $S$ are the vector of conserved quantities, flux vector, and the source vector, respectively. Park's two-temperature model (Park 1987) for thermal nonequilibrium is taken into account. In this model, the translational and rotational temperatures are regarded as a common temperature $T$, while the vibrational temperature of each molecule, electronic excitation temperature of each species, and translational temperature of free electron are regarded as another common temperature $T_V$. The vector of conserved quantities $U$ is as follows:

$$U = (\rho, \rho u, \rho e, \rho e_V)^T.$$
where \( \rho_s \) is the density of each species, \( u_j \) is a flow velocity, \( e \) is the total energy of per unit mass, and \( e_V \) is the summation of the vibrational energy of each molecule, the translational energy of free electron, and the electronic excitation energy per unit mass. The vibrational energy of each species is calculated based on the harmonic oscillator model, while the first two terms of the partition function are taken into account for the electronic excitation energy of each species.

The relaxation time for the translational-vibrational energy exchange is calculated using the semi-empirical correlation proposed by Millikan and White (Millikan & White 1963) with the correction term suggested by Park (Park 1987). As for the molecular energy transfer process in which a certain amount of energy is removed at dissociation or is added at recombination of molecules, the amount of the energy is set to be 30% of the dissociation energy of each molecule (Sharma et al. 1988), which is called "preferential dissociation model" (Park 1990).

For chemical reactions, we considered 11 species for air consisting of \( \text{N, O, N}_2, \text{O}_2, \text{NO}, \text{N}^+, \text{O}^+, \text{N}_2^+, \text{O}_2^+, \text{N}_0^+ \), and \( e^- \). As for the rate coefficients for the chemical reactions in a high temperature air, the Park’s reaction set (Park 1990) for air species is considered.

### 2.1 Diffusion models

The existing diffusion models give a value of diffusion coefficient which slightly differs from each other while the difference may have a large impact on the distribution of chemical species near the wall and, therefore, on the convective heat flux. In this study, we took account of the three models which are currently widely-used. The brief descriptions of each model are given in the following section. The thermal conductivities and viscosity are calculated by the method written in the reference (Gnoffo et al. 1989) with tabulated data of the reference (Gupta et al. 1990).

**Stefan-Maxwell model**

The Stefan-Maxwell model is believed to be the most sophisticated model for the multi-species diffusion coefficients. In the model, the mole fraction gradient is represented by means of the diffusion flux and the diffusion coefficient in a following way;

\[
\nabla x_i = \frac{M}{\rho} \sum_{j \neq i} \left( \frac{x_i J_j}{M_j D_{ij}} - \frac{x_j J_i}{M_i D_{ij}} \right),
\]

where \( J_i \) and \( D_{ij} \) are the diffusion flux of species \( i \) and the binary diffusion coefficient for a pair of species \( i, j \) respectively.

Here we introduce the effective diffusion coefficient \( D_{im} \) for species \( i \) is defined in the following form,

\[
\frac{1 - x_i}{D_{im}} = \sum_{j \neq i} \frac{x_j}{D_{ij}}.
\]

Then eq. (3) can be rewritten to solve for the diffusion flux of species \( i \) in the following form;

\[
J_i = -\rho \frac{M_i}{M (1 - x_i)} \nabla x_i + \frac{c_i}{(1 - x_i)} D_{im} \sum_{j \neq i} \frac{M_j J_j}{M_j D_{ij}}.
\]
Since either equation (3) or (5) is a set of \((n - 1)\) equations for \(n\) species, a closure equation is required to solve them. The closure equation is given by the mass conservation equation:

\[
\sum_i J_i = 0
\]  

(6)

A set of equations based on eq. (3) and eq. (6) must be solved simultaneously. In this study, this set of equations is solved by an iterative method. To accomplish this, we employ the following equation instead of the closure equation eq. (6);

\[
J_i^{N+1} = J_i^N - c_i \sum_j J_j^N
\]  

(7)

where the superscript \(N\) means the number of iteration. In this iterative method, we solve the following equation for eq. (5);

\[
J_i^{N+1} = -\rho \frac{M_i}{M} \frac{D_{im}}{1 - x_i} \nabla x_i + \frac{c_i}{1 - x_i} D_{im} \sum_{j \neq i} \frac{M_j J_j^N}{M_i D_{ij}},
\]  

(8)

being combined with eq. (7). After sufficient converge is attained starting from an initial guess for \(J_i^0\), the solution satisfies a set of equations; i.e., eq. (5) and eq. (6). This iteration was repeated for 10 times typically.

**Yos model**

Yos model is based on an analogy with the binary diffusion which is given in terms of mole fraction;

\[
J_i = -\rho \frac{M_i}{M} \left(1 - \frac{c_i}{1 - x_i}\right) D_{ij} \nabla x_i.
\]  

(9)

In the Yos model, the binary diffusion coefficient \(D_{ij}\) for a pair of species \(i, j\) is replaced by the effective diffusion coefficient, \(D_{im}\). Thus, the diffusion mass flux for species \(i\) for the Yos model is written in the following form,

\[
J_i = -\rho \frac{M_i}{M} \left(1 - \frac{c_i}{1 - x_i}\right) D_{im} \nabla x_i
\]

\[
= -\rho \frac{M_i}{M} \left(\frac{1 - c_i}{\sum_{j \neq i} (x_i/D_{ij})}\right) \nabla x_i.
\]  

(10)

where \(D_{im}\) is calculated using eq. (4).

To see a relation between the Yos model and the Stefan-Maxwell model, eq. (5) can be rearranged in the following form,

\[
J_i = -\rho \frac{M_i}{M} \left(1 - \frac{c_i}{1 - x_i}\right) D_{im} \nabla x_i + \frac{c_i}{1 - x_i} D_{im} \sum_{j \neq i} \left(\frac{M_j}{M} \nabla x_j + \frac{M_i J_j}{M_j D_{ij}}\right).
\]  

(11)

As it shows, the difference between the Yos model and the Stefan-Maxwell model arises from the second term of eq. (11). (Sutton & Gnoffo 1998)
In the Lee model, the binary diffusion coefficient in eq. (10) is approximated by using the common diffusion coefficient $D$, (Cander & MacCormack 1988)

$$\frac{1-x_i}{D} = \sum_{j \neq i} \frac{x_j}{D_{ij}}$$

(12)

where $D$ is calculated by the following relation,

$$D = \frac{\mu}{\rho S_c}.$$  

(13)

In this study, the Schmidt number, $S_c$, is assumed to be constant and is set to be 0.5.

Using this common diffusion coefficient $D$ and eq. (10), the diffusion flux of species $i$ for the Lee model is defined as follows,

$$J_i = -\rho \frac{M_i}{M} \left( \frac{1-c_i}{1-x_i} \right) D \nabla x_i.$$

(14)

Comparison of eq. (10) with eq. (14) tells that the Lee model is an approximation of the Yos model, in that $D_{im}$ in the Yos model is replaced by a common value of $D$.

3. Numerical methods

To solve eq. (1), we employed the Advection Upstream Splitting Method (AUSM) type scheme (Liou & Steffen 1993; Wada & Liou 1994). This type of scheme can capture a stationary discontinuity with negligible numerical dissipation and is robust enough to calculate the shock waves and expansion waves. Additionally, this scheme is of a flux splitting type, which is suitable to its application to a large system of equations. As for the stiffness problem related to the strong dissociation and ionization reactions, a diagonal implicit method (Otsu et al. 1998; Bussing & Murman 1985; Eberhardt & Imlay 1990) was employed. The total number of the computational grid was 1800 points, 30 points along the body surface and 60 points along the line normal to the body surface.

3.1 Calculation cost

All the calculations were performed on the computer with a CPU chip of Alpha 21264/600 MHz and 256 MB RAM. A steady solution is obtained after a sufficient iteration based on the time-marching method.

To compare the performance of the various models, the accuracy of the calculated result is of a primary importance. However the computational cost to accomplish it is also important. To measure the computational cost, the CPU time necessary to carry out 1000 iterations was compared for the three models. Each CPU time was shown on Table 1. From this table, the CPU time of the Stefan-Maxwell model is found to be about 2 times larger than that of the Lee model, while the Yos model requires almost the same cost with the Lee model.

4. Results and Discussions

As for a nominal situation for the flow field calculation, we consider the flight condition of MUSES-C mission. In the flight condition, we focus on the flight condition at which the
reentry capsule encounters the peak convective heat flux; i.e., the reentry flight velocity of 11.6 km/s at the altitude of 64 km. The MUSES-C reentry capsule has a configuration of a sphere cone with a 45-deg. half angle, a nose radius of 20 cm, a sharpened shoulder, and a flat base. The boundary condition at the vehicle surface is imposed in a way that the wall temperature is fixed at 3000 K. At the vehicle surface, we investigate both the non-catalytic wall condition and the full-catalytic wall condition to examine their influence on the effect the diffusion models. Under the non-catalytic wall condition, the concentrations of neutral species are calculated by assuming a vanishing diffusive flux except ions and electron. As for the ions and electron, their concentration at the surface is set to be zero. This is because the electronic neutrality at the surface of the vehicle must be attained. This means that the surface is treated as a catalytic one for the ions and electron even under the non-catalytic wall condition. On the other hand, under the full-catalytic wall condition, the concentrations of all the species are set to become the same value as the free stream condition.

4.1 Flow characteristics on the stagnation line

In this section, a brief description of flow characteristics at the stagnation region is given. Here we focus on the nominal flight condition; i.e., the reentry flight velocity of 11.6 km/s at the altitude of 64 km. As for the boundary condition at the surface, the non-catalytic wall condition is imposed. The temperature distribution along the stagnation line is shown in Fig 1. The translational-rotational temperature, $T_t$, reaches the maximum value at $X = 14$ mm, while the vibrational-electronic temperature, $T_v$, is still much lower than $T$. $T_v$ begins to be equilibrated around at $X = 6$ mm and continues to be equilibrated until the surface. On the contrary, the thermal nonequilibrium is observed at the region adjacent to the equilibrium region; i.e., from $X = 16$ mm to $X = 6$ mm. The equilibrated temperature amounts up to about 12000 K.

Figure 2 shows the distribution of chemical species. From these figures, we can see that N$_2$ and O$_2$ molecules dissociate rapidly and, successively, the generation of NO molecule, the atomic nitrogen and oxygen, and the ionization of the molecules such as N$_2$, O$_2$ and NO, occur rapidly in the thermal nonequilibrium region. Then, after the rapid generation, the molecular species rapidly begins to dissociate. In the thermal equilibrium region, the ionic atoms N$^+$ and O$^+$ are created. The mass fraction of atomic ions such as N$^+$ and O$^+$ amount up to around 0.14 and 0.03 respectively. These values are relatively high compared to the one expected for the low reentry speed condition. Besides the atomic ions, the dissociation proceeds more extensively in this speed range than in the low reentry speed range.

Effect of diffusion models on the flow properties near the surface

Now, we will see the effect of the each diffusion models on the flow characteristics. The results shown in this section are for the nominal reentry flight condition with non-catalytic wall condition. Figure 3 shows the temperature distributions near the surface. In the region far from the surface, the temperature for the Lee model is slightly (about 500 K) lower than

<table>
<thead>
<tr>
<th>Model</th>
<th>Lee</th>
<th>Stefan-Maxwell</th>
<th>Yos</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU time [s]</td>
<td>663.20</td>
<td>1393.82</td>
<td>660.94</td>
</tr>
</tbody>
</table>
that of other two diffusion models while, in the region close to the surface, the difference among the diffusion models is negligibly small. This suggests that the heat flux derived from the temperature gradient is almost independent on the diffusion model. In contrast to the temperature distribution, the behavior of the mass fraction of chemical species depends on the diffusion model as shown in Fig. 4 where the distribution of mass fraction of N\textsuperscript{+} is depicted for the three diffusion models. The distribution of N\textsuperscript{+} near the surface for the Lee model clearly differs from that of other two models, and is steeper than that in the other models. This suggests that the heat flux derived from the diffusion of ionic species may depends on the model. We will argue about this subject in the following sections.
4.2 Heat flux estimation at the stagnation

The aerodynamic heat flux is a sum of the contribution from the translational and vibrational temperature gradients, the diffusion of enthalpy of ions/electrons, and the other neutral species. The influence of the diffusion model appears differently in each contribution and also is affected by various conditions such as the wall catalysity and flight conditions. In the following sections, we will investigate the influence of the diffusion model on the heat flux under various conditions.
Effect of wall catalysity

Under the non-catalytic wall condition, the main source of the convective heat flux is the conduction of energy due to the gradients of $T$ and $T_v$ as shown in Fig. 5, even though a contribution from the diffusion of enthalpy (that is, the diffusion of ions/electrons) still exists. In both the Stefan-Maxwell model and the Yos model, the contribution from the diffusion of enthalpy is negligibly small and almost the same amount of heat flux is predicted since their temperature profiles near the surface are almost identical as discussed above. In the Lee model, however, the contribution of the diffusion is not small and the heat flux higher than the other models is predicted since the contribution of the temperature gradients is almost the same as that in the other models. That is, the difference between them arises from the heat flux related to diffusion of ions/electrons.

Under the full-catalytic wall condition, as can be seen in Fig. 6, the heat flux contributed from the diffusion of the chemical species, especially the diffusion of neutral species, becomes significant. This is because, near the surface, the concentration of neutral species is much larger than that of ions, and the temperature distribution is almost unaffected by the wall catalysity. On the contrary, the contribution from the temperature gradient is almost the same as the one predicted in the non-catalytic wall condition. Because of this, the heat flux under the full-catalytic wall condition is much larger than that under the non-catalytic wall condition. In the Lee model, the contribution from the diffusion is larger than that in the other models even though the ions/electron contribution becomes small being compared to that under the non-catalytic wall condition. Hence, the Stefan-Maxwell model and the Yos model gives a similar value for the heat flux, while the one for the Lee model is larger than the others.

Effect of the reentry flight velocity

Besides the wall catalysity, it is expected that the variation of flight condition may affect the appearance of the model dependency since the variation of the flight condition gives rise to the variation of flow characteristics which may affect the aerodynamic heat flux. In this section, we investigate the behavior how the appearance of the model dependency depends on the flight condition. As for the reentry flight condition, the reentry flight velocity and the atmospheric density are considered.

To examine the effect of flight velocity, the reentry flight velocity is varied from 9.0 km/s to 13.0 km/s including the nominal value inbetween, while the density is fixed as a nominal value.

From Fig. 7, it is observed that the larger the reentry flight velocity is, the larger the convective heat flux is. This is the case in all the diffusion models. Though the result by the Stefan-Maxwell model and the Yos model shows a similar trend with the increasing velocity, the result by Lee model differs from the others. The discrepancy between them becomes larger with the larger flight velocity. This behavior is observed not only in the case of the non-catalytic boundary condition but also in the case of the catalytic boundary condition. As discussed above, the discrepancy between the Lee model and the other models is derived from the contribution of the diffusion of enthalpy of the chemical species. Hence this increase in the discrepancy is because the number of chemical species of dissociated air becomes significant with the increasing flight velocity, since the larger the flight velocity is, the stronger the shock wave is and, behind the stronger shock wave, the chemical reactions proceeds more extensively.

As mentioned above, we can see that the difference between the Yos model and the Stefan-Maxwell model is very small. This means that the Yos model can predict the convective heat
Fig. 5: Comparison of convective heat flux under the non-catalytic wall condition.

Fig. 6: Comparison of convective heat flux under the full-catalytic wall condition.

flux with almost the same accuracy of the Stefan-Maxwell model under the flight velocity range between 9.0 km/s and 13.0 km/s. Also it should be mentioned that, in a low speed range such as 9 km/s, the discrepancy between the Lee model and the other models is reasonably small while the discrepancy can not be neglected in the reentry speed range inherent to the super-orbital reentry. That is, in a low speed range, the Lee model can be acceptable while, in the higher reentry speed, the Lee model is hardly acceptable.
Effect of the atmospheric density

In this section, we will examine the effect of the atmospheric density on the heat flux. To this aim, the atmospheric density was varied from $1.0 \times 10^{-4}$ kg/m$^3$ to $4.0 \times 10^{-4}$ kg/m$^3$ including the nominal value in between, while the reentry flight velocity is fixed as the nominal value. The variation of the atmospheric density corresponds to the variation of the flight altitude.

The heat flux at the stagnation increases with the increasing atmospheric density as shown in Fig. 8. Though the result by the Stefan-Maxwell model and the Yos model reasonably agrees to each other, the result by the Lee model differs from the others. The discrepancy between
them, however, shows only a slight dependency on the increase of the density. This is the case not only in the case of the catalytic wall condition but also in the case of the non-catalytic wall condition.

5. Conclusion

In this study, we assessed the models for diffusion coefficients in a view point of the application to simulate the hypersonic reentry heating environment. The nominal flight condition for the assessment is the reentry speed of 11.6 km/s at the altitude of 64 km which corresponds to the flight condition for the peak aerodynamic heating during the super-orbital reentry. Three diffusion models; the Stefan-Maxwell model, the Yos model, and the Lee model, are evaluated. The Stefan-Maxwell model is the most sophisticated while the Yos model is an approximation of the Stefan-Maxwell model. The Lee model is a further approximation of the Yos model, and is the simplest among them.

In the nominal flight condition case, under both the non-catalytic wall condition and the full-catalytic wall condition, the Lee model shows a discrepancy with the other two models and gives a higher heat flux. On the contrary, the Stefan-Maxwell model and the Yos model show a reasonably good agreement between them. The discrepancy between the Lee model and the others is derived from the extent of the contribution of diffusion of enthalpy of the chemical species.

In order to investigate the effect of the reentry flight condition on the heat flux, the effect of the reentry flight velocity and the atmospheric density was investigated. The discrepancy between the Stefan-Maxwell model and the Yos model is reasonably small in all the circumstance. On the other hand, there is a discrepancy between the Lee model and the others. The discrepancy between the Lee model and the others increases with an increase of the velocity while the discrepancy shows only a negligible dependency on the atmospheric density. This increase of the discrepancy is attributed to the increase of the chemical species of dissociated air with the increase of the velocity. Because of this, even the Lee model is acceptable in a low reentry speed range such a reentry from LEO. However the Lee model is hardly acceptable for an application to the higher velocity reentry such as a super-orbital reentry.

As for the calculation cost, the Stefan-Maxwell model is about two times more expensive than the other two models.

From these results, we can conclude that, in a view point of estimating the heat flux for the super-orbital reentry flight vehicle with a reasonably accuracy and a reasonably computation cost, the Yos model is the most recommendable among the three models considered in this study.

According to the present investigation, the diffusion model has a significant influence on the accuracy of the prediction for the heat flux. This, in return, suggests that we should pay more attention to the selection of the models for other transport properties and the further investigations in modeling the transport phenomenon are important for the accurate estimation of the heat flux.

REFERENCES


