Effect of Transport Coefficients on Aero-thermal Predictions of Re-entry Flows

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Abstract

The effect of viscosity coefficient on aero-thermal prediction of re-entry flows is studied by computing the flowfield with different formulations for individual species viscosity. Blottner viscosity model and collision integral method are used to calculate the species viscosity. The surface properties of FIRE II re-entry capsule at 35 km altitude computed using the above two viscosity formulations are compared with the in-flight measurements. The stagnation point heating rate predicted by collision integral method is 10% higher than that given by Blottner model. Afterbody heat transfer rate computed by both formulations are within the scatter of flight data. Shock position predicted by both methods differ slightly at the shoulder region. However their effect on surface pressure is minimal.

I Introduction

In a re-entry flowfield the high temperatures at the bow shock wave initiate the excitation of vibrational modes, dissociative chemical reactions and ionization in the gas. Thus accuracy of numerical prediction of aero-thermal loads on re-entry vehicles depends on the accuracy of the physical models, used to describe these high temperature effects. One critical aspect of physical modeling of re-entry flowfields is the computation of transport properties of dissociated gas i.e. viscosity, thermal conductivity and diffusion coefficients of the gas mixture. These parameters model the viscous transport of momentum, energy and mass in the flowfield. Hence appropriate relations for transport properties should be used for accurate computation of flow gradients at the shock wave and in the viscous dominated regions i.e. boundary layer and separation regions.

The problem of finding the viscosity coefficient of a mixture involves calculation of viscosity coefficients of individual species and then computing the mixture coefficient from the individual species data using mixing rules. Palmer et.al¹ compare the accuracy and computational efficiency of most commonly used mixing rules in the temperature range of 200 K to 20000 K. In this work viscosity of individual species is computed using the collision integral formulation which can be obtained form the principles of kinetic theory of gases. Other commonly used relation for individual species viscosity is Blottner curve fit correlation.² However its validity to the re-entry flowfields with temperatures above 10000 K

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is questionable.\textsuperscript{3} Hence collision integral based method is used in the numerical formulation of re-entry flows if temperatures are very high. However thorough study of viscosity relation of collision integral method and Blottner model is required for reliable prediction of surface properties for re-entry flows.

The objective of the present work is compute the re-entry flowfield with individual species viscosity relation given by Blottner model and collision integral method. The surface quantities obtained from the two formulations are compared with the flight data. Flowfield over FIRE II re-entry capsule at 35 km altitude trajectory point\textsuperscript{4} is chosen for this study and corresponding freestream conditions are $\rho_\infty = 0.0082 \text{ Kg/m}^3$, $U_\infty = 4950 \text{ m/s}$, $T_\infty = 237 \text{ K}$ $M_\infty = 16$ and $T_w = 553.3 \text{ K}$. The flowfield has been computed with the Blottner viscosity model and detailed description of the computed flowfield and comparison of surface properties with the flight data are given Ref. 5.

The outline of the paper is as follows. The details of the simulation methodology and viscosity relations of Blottner model and collision integral method are given next. Description of the computed flowfield, composition of the gas at shock wave and boundary layer and comparison of the surface properties obtained by above two viscosity relations are presented subsequently. Finally, conclusions drawn from the current work are presented.

II Simulation Methodology

The simulation methodology used in the present work is same as that used in Ref 4, and a brief summary is given below. The chemically reacting turbulent hypersonic flow around the FIRE II re-entry configuration is simulated by solving the Reynolds-averaged Navier-Stokes (RANS) equations along with the species conservation equations and a thermal non-equilibrium model. Air is modeled as a neutral mixture of five perfect species ($N_2$, $O_2$, $NO$, $N$ and $O$) with three dissociation and two exchange reactions. Two temperature model of Park\textsuperscript{6} is used to describe the thermal state of the gas. An additional conservation equation is solved for the vibrational energy of the mixture to account for the thermal non-equilibrium. The Arrhenius rate constants for the chemical reactions are evaluated using curve fits to experimental data by Park.\textsuperscript{6}

The axisymmetric form of the governing equations are discretized using the finite volume approach. Inviscid fluxes are computed using a modified (low-dissipation) form of the Steger-Warming flux splitting approach,\textsuperscript{7} and the turbulence model equations are fully coupled to the mean flow equations.\textsuperscript{8} The method is second-order accurate in both streamwise and wall-normal directions. The viscous fluxes and the turbulent source terms are evaluated using second-order accurate central differenting and the implicit data parallel line relaxation method\textsuperscript{9} is used to obtain steady-state solutions. Spalart-Allmaras (SA) model\textsuperscript{10} is used for turbulence closure.

Viscosity of individual species ($\mu_s$) is computed using Blotter curve fit expression\textsuperscript{2} which is given below.

$$\mu_s = 0.1 \exp[(A_s \ln T + B_s) \ln T + C_s]$$

(1)

Where $A_s$, $B_s$, $C_s$ are the curvefit coefficients for species and are given in Table 1. $T$ is the mixture
Table 1: Viscosity coefficients for Blottner model (Eq. 1)

<table>
<thead>
<tr>
<th>Species</th>
<th>$A_s$</th>
<th>$B_s$</th>
<th>$C_s$</th>
<th>$D_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2$</td>
<td>0.0268142</td>
<td>0.3177838</td>
<td>-11.3155513</td>
<td></td>
</tr>
<tr>
<td>$O_2$</td>
<td>0.0449290</td>
<td>-0.0826158</td>
<td>-9.2019475</td>
<td></td>
</tr>
<tr>
<td>$NO$</td>
<td>0.0436378</td>
<td>-0.0335511</td>
<td>-9.5767430</td>
<td></td>
</tr>
<tr>
<td>$N$</td>
<td>0.0115572</td>
<td>-0.6031679</td>
<td>-12.4327495</td>
<td></td>
</tr>
<tr>
<td>$O$</td>
<td>0.0203144</td>
<td>0.4294404</td>
<td>-11.6031403</td>
<td></td>
</tr>
</tbody>
</table>

Table 2: Curve fit coefficients for collision integrals (Eq. 3)

<table>
<thead>
<tr>
<th>Species</th>
<th>$A_s$</th>
<th>$B_s$</th>
<th>$C_s$</th>
<th>$D_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2$</td>
<td>0.008796</td>
<td>-0.198792</td>
<td>1.302289</td>
<td>-0.000054</td>
</tr>
<tr>
<td>$O_2$</td>
<td>0.007817</td>
<td>-0.183309</td>
<td>1.226963</td>
<td>-0.000085</td>
</tr>
<tr>
<td>$NO$</td>
<td>0.007123</td>
<td>-0.175471</td>
<td>1.212750</td>
<td>-0.000089</td>
</tr>
<tr>
<td>$N$</td>
<td>0.006099</td>
<td>-0.157690</td>
<td>1.080707</td>
<td>-0.000099</td>
</tr>
<tr>
<td>$O$</td>
<td>0.007543</td>
<td>-0.183804</td>
<td>1.191239</td>
<td>-0.000086</td>
</tr>
</tbody>
</table>

translational temperature. The collision integral relation for individual species viscosity is given by\(^1\)

$$\mu_s = 0.1 \times 2.6639e - 5 \frac{\sqrt{M_s T}}{\sigma^2 \Omega^{(2,2)*}_{ss}}$$

(2)

Where $M_s$ is molecular weight of species $s$ (gm/mole), $\sigma$ ($A_s$, angstrom) is rigid sphere collision diameter and $\Omega^{(2,2)*}_{ss}$ is reduced viscosity collision integral. Viscosity given by both formulations (Eq. 1 and 2) is in SI units i.e. kg/m.sec. Wright et al.\(^11\) summarizes the collision integrals data for all possible binary interactions in air for earth re-entry flows from the latest available data. The data is presented at the discrete temperature. Hence a curve fit to the given data as a function of temperature is required to obtain the collision integral values. In the present work a standard logarithmic form\(^3\) is assumed and is given below.

$$\sigma^2 \Omega^{(2,2)*}_{ss} = \exp(D_s) \cdot T^{A_s \ln(T)^2 + B_s \ln(T) + C_s}$$

(3)

The constants $A_s$, $B_s$, $C_s$, $D_s$ can be obtained by least square curve fit method. For the above logarithmic form, the least square method results in the following system of equations, which can be solved for $A_s$, $B_s$, $C_s$, $D_s$.

$$\begin{bmatrix}
\sum X_i^6 & \sum X_i^5 & \sum X_i^4 & \sum X_i^3 & \sum X_i^2 & \sum X_i \\
\sum X_i^5 & \sum X_i^4 & \sum X_i^3 & \sum X_i^2 & \sum X_i & 1
\end{bmatrix}
\begin{bmatrix}
A \\
B \\
C \\
D
\end{bmatrix}
= \begin{bmatrix}
\sum Y_i X_i^3 \\
\sum Y_i X_i^2 \\
\sum Y_i X_i \\
\sum Y_i
\end{bmatrix}$$

(4)

where $\sum$ refers to the summation over given data points and

$$X_i = \text{log}(T_i), \quad Y_i = \text{log}(\sigma^2 \Omega^{(2,2)*}_{ss})_i$$

(5)
The constants $A$, $B$, $C$, $D$ for the five species computed by above method are listed in Table 2.

## III Results

Figure 1 shows the viscosity computed from the collisional integral method (Eq. 2) to that given by the Blottner model (Eq. 1). Over a wide range of temperature (upto 20000 K), species viscosity predicted by collision integral method for $O_2$, $O$ and $NO$ is higher than that of Blottner model. At temperatures around 5000 K, viscosity of these species given by collision integral method is higher by 10% than the Blottner model. For temperatures below 5000 K, viscosity of $N_2$ and $N$ computed by both models is within 5%. However above 5000 K, collision integral method predicts lesser value than that given by Blottner model. The deviation between the two formulations is highest for $N_2$ among the all species with collision integral method predicting 15% lesser value compared to that of Blottner model at 10000K. In a typical re-entry flowfields the boundary layer edge temperatures are around 5000 K to 10000 K. Hence the difference in prediction of viscosity between the two formulation at these temperatures can lead to the difference in the computed surface quantities. The results presented below highlights this point further.

Before presenting the comparison of surface properties that are obtained by different formulation of viscosity, a brief description of the re-entry flowfield is given. The main features of flowfield in terms of Mach number contours over FIRE II capsule at Mach 16 are depicted in Fig. 2. The detached bow shock ahead of the forebody decelerates the flow and causes sudden rise in temperature of the gas at the shock. These high temperatures at the shock wave, excite the internal energy modes and chemical reactions in the gas, resulting in non-equilibrium flow downstream of the shock. The temperature in the forebody stagnation region is about 5700 K. The flow on the entire forebody is subsonic with the Mach

![Figure 1: Ratio of species viscosity computed from the collision integral method (Eq. 2) to that of Blottner model (Eq. 1)](image-url)
number approaching unity close to the first expansion corner. Flow expansion at the first corner results in decrease of temperature to 4100 K. Flow expansion around the second corner further decreases the temperature to about 1800 K.

Boundary layer separates immediate after the second corner and forms the recirculation region which consists of a single toroidal vortex. Flow in the separation bubble is subsonic with vortex core at temperature about 5800 K. The temperature in the outer inviscid region of the afterbody is about 2000 K and corresponding Mach number is $\sim 3.5$. A free shear layer originating from the separation point, separates the inner recirculation region and outer inviscid flow. The outer inviscid flow is turned to freestream direction by a re-compression shock at the neck region which increases the temperature of the gas to about 4900 K.

Gas composition at the shock wave along the stagnation stream line is shown in Fig. 3(a). Due to the high temperatures at the shock wave, oxygen molecules are mostly dissociated in the post-shock region with an atomic oxygen mass fraction of 0.22. NO is formed behind the shock to a maximum level of 8%. It decreases to 2% in the post-shock region. The exchange reactions results in increase of $Y_{N}$ up to 0.04 and decrease of $Y_{N_{2}}$ to 0.71. The gas composition in majority portion of the forebody is approximately equal to that of post-shock values on stagnation stream line. The flow expansion at the shoulder results in slight increase of $Y_{N_{2}}$ and $Y_{O}$ with a corresponding decrease in $Y_{N}$ and $Y_{NO}$. The gas composition in the afterbody inviscid expansion region is primarily composed of $N_{2}$ and $O$ with mass fraction of 0.75 and 0.23 respectively. Slight changes in the mass fraction of $N_{2}$, $N$ and $NO$ are observed in the separation bubble due to chemical reactions in the hotter vortex core region.

Figure 3(b) illustrates the variation of gas composition in the thermal boundary layer along the stagnation stream line. Local thermal boundary layer thickness is used to non-dimensionalize the wall normal distance. Hence $l/\delta = 0$ represents wall and $l/\delta = 1$ corresponds to the thermal boundary layer edge. In the boundary layer mass fraction of atomic species i.e. $O$ and $N$ decrease and a corresponding increase in mass fractions of $O_{2}$ and $N_{2}$ can be noticed. $Y_{NO}$ also increases from 0.02 at edge of boundary layer to 0.05 at wall. The gas composition changes primarily due to the recombination reactions.

Figure 4(a) shows the computed surface heat transfer rate on the forebody as a function of the normalized arc-length ($s/D$) measured from the nose of the vehicle. $s/D = 0$ represents nose stagnation point and $s/D = 0.52$ is the first expansion corner. Heat transfer rate varies gradually on the forebody with a maximum value of 219 W/cm$^2$ at the nose. The stagnation-point heating rate matches the theoretical estimate of Fay and Riddell\textsuperscript{12} (shown by the symbol in Fig. 4(a)). At the expansion corner heating rate has a local peak followed by a sharp decrease as the gas temperature drops due to flow expansion. The afterbody heat transfer rate is shown in Fig. 4(b). The extent of the conical frustum and flat base are identified in the figure. The expansion corners are marked by local peaks in the heat transfer rate. In between the two expansion corners, the heating rate show a monotonic increase from the separation point at the shoulder to the base corner. The base stagnation point heating rate is 22.48 W/cm$^2$, which is 10.3% of the corresponding nose stagnation point value. The above results are computed using the Blottner viscosity model.
The heating rate obtained from the Blottner model is compared with that obtained from the collision integral method in Fig. 6. Collision integral formulation predicts higher heat transfer rate on majority portion of the forebody with a maximum difference at the nose stagnation point. The predicted stagnation point heating rate by collision integral method is higher than that of Blottner model by 9.44%. The Fay and Riddell estimate of stagnation point heat transfer rate is closer to the Blottner model value than that of collision integral method. The difference between the two models decreases away from the nose stagnation point.

Similar to forebody, on the afterbody also collision integral method predicts higher heating rate. Both models predicts approximately same value of heating rate at the beginning of conical frustum on afterbody. Difference between the heating rate increases as we move towards to base stagnation point. Heat transfer rate predicted by collision integral method at the base stagnation point is 16% higher than that of Blottner model. In-flight measurement of heating rate also shown in Fig. 5(b). The heat transfer rate computed by the both models is with in the scatter of flight data on the conical frustum. At the chosen freestream conditions, the temperature of the gas at the edge of the forebody boundary layer is around 5500 K. At this range of temperatures, collision integral method predicts higher viscosity for the species \(O_2\), \(NO\) and \(O\) compared to the Blottner model (see Fig. 1). However for atomic and molecular nitrogen both models predicts approximately same values of viscosity at these temperatures. The gas composition in the forebody boundary layer is primarily composed of \(N_2\) and \(O_2\). Higher viscosity of \(O_2\) predicted by collision integral method leads to the higher heating rate on the forebody. The temperature of the gas, in the near wall region of the afterbody, progressively increases from 2000 K at the beginning of conical frustum to about 4500 K at base stagnation point and the gas is composed of \(N_2\) and \(O\). The difference between the viscosity predicted by both models at around 2000 K is less than 5%. Hence both models predicts approximately same level of heating rate at the beginning of conical frustum. For oxygen atoms, at around 3000 K, the collision integral method predicts 10% higher viscosity than Blottner model. Hence collision integral methods predicts higher heating rate near the base region.

Figure 6(a) shows temperature profile on a body normal line at the shoulder region. Both models predicts the peak translation temperature about 7100 K. The figure also depicts the difference the prediction of shock detachment distance. The value computed by the collision integral method is 3% higher than that of Blottner model value. However at the stagnation stream line both models predicts the identical shock detachment distance. Figure 6(b) shows that the difference between the forebody normalized wall pressure computed by both models is negligible. Although minor changes in the shock detachment distance are observed, its effect on computed surface pressure is negligible. It is observed that the computed surface pressure by both models is identical on the afterbody. However the comparison is omitted for the sake of brevity.

**IV Conclusions**

Flowfield over FIRE II re-entry capsule at 35 km altitude trajectory point is computed with the
individual viscosity, given by the Blottner model and collision integral method. The computed surface properties obtained from the both models are then compared with the in-flight measurement to assess the effect of viscosity. At around 2000 K, viscosity computed by both models is approximately same. However for temperatures above 2000 K, collision integral method predicts higher values of viscosity for $O_2$, $NO$ and $O$ and lower values for $N_2$ and $N$. This difference in prediction of viscosity leads to changes in computed heating rate by both models. The nose and base stagnation point heating rate predicted by collision integral method is higher than that given by 10% and 16% respectively. However the heating rate computed by both models on the afterbody conical frustum are within the scatter of in-flight measurement. Surface pressure predicted by both models is almost identical on entire vehicle surface.
Figure 4: Heat transfer rate computed using Blottner viscosity model: (a) forebody, and (b) afterbody.

Figure 5: Comparison of heat transfer rate obtained by Blottner model and collision integral method: (a) forebody, and (b) afterbody.

References


Figure 6: Effect of viscosity coefficient (a) on shock wave position at shoulder region and (b) normalized pressure on forebody


