Analysis of Thermochemical Nonequilibrium Ablation Flow for a Hypersonic Hemispherical Nose

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Abstract. The thermal protection materials enveloping hypersonic vehicles ablate. This paper develops a numerical methodology of thermochemical nonequilibrium flow and structure temperature field to study the key flow and structure parameters of a hypersonic hemispherical nose under the condition of carbon-based thermal protection material ablation. The multi-species chemical reaction model of flow field and the corresponding numerical algorithm are constructed. Oxidation and sublimation ablation process are considered in ablation model coupled with flow field solver by gas-solid interaction method. The computational results of a hemispherical nose indicate that carbon-based thermal protection material ablation has significant effects on thermochemical nonequilibrium flow. Details of the ablation flow characteristics are reported to highlight the influences of ablation on microcosmic reaction species and macroscopic flow parameters including shock wave position, pressure and temperature.

1. Introduction
Serious aerodynamic heating will lead to the ablation of carbon-based thermal protection material on the surface of hypersonic vehicles the aircraft, which affects the characteristics of thermochemical nonequilibrium flow field. The ablation mechanism of thermal shielding materials and the characteristics of thermochemical nonequilibrium ablation flow field of hypersonic vehicle have been studied extensively. Based on JANAF sublimation carbon group model[1], two kinds of surface ablation models named after chemical equilibrium model[2] and finite rate model[3, 4] are developed. The collision integration model and the rate coefficient of forward and reverse reaction are measured to simulate the ablation flow field of the hypersonic vehicle using the carbon-phenolic thermal protection materials[5]. Considering the pyrolysis effect of the resin inside the carbon-phenolic ablation material at a lower temperature, a more accurate ablation reaction model is developed[6]. Coupled with the relationship of mass and energy balance on the ablation surface, the numerical results based on NS equations are in good agreement with experiment values[7]. Multi-component chemical reaction model is used to calculate polypropylene ablation flow field of blunt cone re-entry and the influence of ablation products on electron number density in wake area is detailed studied[8,9]. The prediction of continuous ablation and heat transfer in the whole re-entry process is realized by aerodynamic engineering estimation method and nonlinear heat conduction equation[10].

The objective of this paper is to develop appropriate simulation methods for capturing the key parameters of the thermochemical nonequilibrium ablation flow and reveal the mechanism by which the ablation influences the chemical component characteristics of a hypersonic hemispherical nose.
The two-way coupled effect of flow field and structure temperature field is considered and the ablation flow field is calculated by NS equations to guarantee precision.

2. Thermochemical nonequilibrium reaction model

According to the flight conditions of hypersonic vehicle and the characteristics of carbon-based material, following species may appear in the flow field: O, N, O$_2$, NO, NO+, CO, C$_1$, C$_2$, C$_3$, CN, CO$_2$ and e. In consideration of chemical nonequilibrium, forward reaction rate $k_f$ and backward rate $k_b$ are defined by Arrhenius form:

$$k_f = A_f T^{B_f} e^{-\frac{E_f}{T}}$$  \hspace{1cm} (1)$$

$$k_b = A_b T^{B_b} e^{-\frac{E_b}{T}}$$  \hspace{1cm} (2)$$

The values of $A_f$, $B_f$, $E_f$ and $A_b$, $B_b$, $E_b$ are also shown in Gupta’s air reaction model\[11\] and Blottner’s ablation products reaction model\[12\]. The governing temperatures of reactions are determined by the type of reactions in Park’s model\[13\]. The equations of state and energy conservation for mixed gas are given as:

$$P = \hat{R} \left( \rho \sum_{i=1}^{s} \frac{X_i}{M_i} \rho T + \rho T \frac{c_p}{M} \right)$$  \hspace{1cm} (3)$$

$$E = E_v + E_e + E_{in} + \frac{1}{2} \left( u^2 + v^2 + w^2 \right)$$  \hspace{1cm} (4)$$

According to Wilke's semi-empirical formula, the viscosity coefficient, vibration coefficient and electronic thermal conductivity of mixed gas are given as:

$$\mu = \sum X_i \frac{\mu_{ij}}{\Phi_i}$$

$$\rho = \sum X_i \rho_{ij}$$

$$k_v = \sum X_i k_{ij}$$

$$k_e = \sum X_i k_{ej}$$

$$k = \sum X_i k_{ij}$$  \hspace{1cm} (5)$$

The diffusion coefficients $D_s$ of component $s$ and electron are written as:

$$\rho D_s = \frac{(1-c_s)\mu}{(1-X_s)S_s}$$  \hspace{1cm} (6)$$

$$\rho D_e = M \sum \frac{c_i \rho D_i}{M_i}$$  \hspace{1cm} (7)$$

3. Carbon-based material ablation model

The surface ablations account for both oxidation and sublimation process for different surface temperatures. The ablation reaction rate is affected by two factors: one is the rate at which oxygen diffuses to the wall or the material sublimation product diffuses to the air, the other is the rate at which the material reacts with the air.

The oxidation process is:

1) $2C + O_2 \rightarrow 2CO$

2) $C + O \rightarrow CO$

The chemical reaction using JANAF sublimation model is:

1) $jC \rightarrow C_j (j = 1, 2, 3)$

2) $C + N \rightarrow CN$

3) $2C + N_2 \rightarrow 2CN$

4) $C + O \rightarrow CO$
The mass ablation rate $\dot{m}_{\text{m}}$ of carbon-based material contains the mass loss rate $\dot{m}_{\text{c}}$ caused by ablation and the mass loss rate $\dot{m}_{\text{t}}$ caused by mechanical denudation. The ablation degradation rate and mechanical denudation factor are presented respectively as:

$$v_{\text{m}} = \frac{\dot{m}_{\text{m}}}{\rho}$$  \hspace{1cm} (8)

$$f_{\text{t}} = \frac{\dot{m}_{\text{t}}}{\dot{m}_{\text{c}}}$$  \hspace{1cm} (9)

where

$$f_{\text{t}} = \begin{cases} 1.0 & P < 20.26 \times 10^5 \text{ Pa} \\ 1.2 & P \geq 20.26 \times 10^5 \text{ Pa} \end{cases}$$  \hspace{1cm} (10)

4. Numerical Algorithm
The flow field governing equations are calculated by Advection Upstream Splitting Method by Pressure-based Weight function[14] (AUSMPW+) while the diffusion terms are central difference. The implicit Lower-Upper Symmetric Gauss-Seidel Relaxation[15] (LU-SGS) is employed as time marching algorithm. Besides, the structure temperature field is solved by heat balance method and the time marching algorithm is explicit Runge-Kutta method[16].

The coupled solving procedure of ablation flow field and structure temperature field is presented as:

1. Calculate the thermochemical non-equilibrium flow field and obtain heat flux, temperature, pressure and mass fraction of each chemical reaction element at fluid-solid interface.

2. Use the results in step 1 as boundary conditions to calculate structure heat transfer and ablation reaction.

3. After structure temperature field marches 10 s, the ablation products and interface temperature are applied as the boundary conditions to calculate the chemical non-equilibrium ablation flow field at that moment.

4. The characteristics of flow and temperature fields at different time are obtained by repeated iteration of interface information.

5. Results and discussion
The flight conditions are given in Table 1 and the hemispherical nose geometry with the radius of 0.5 m are shown in Figure 1. The computational grid contains two regions: flow field in blue and structure temperature field in red. As a compromise between accuracy and computational cost, the grid for flow field comprises 3.5 million cells and the uniform grid for structure temperature field is 0.3 million.

| Altitude, km | Velocity, m/s | Mach No. | Angle of attack, degree | Temperature, K | Time, min |
|-------------|--------------|---------|------------------------|----------------|----------|
| 70          | 6000         | 20.2    | 0                      | 220            | 20       |
The flow field without ablation is firstly studied under non-catalytic wall condition and the species mass fraction distribution is given in Figure 2. O₂ almost fully dissociates behind the shock and part of it forms NO with N₂. Parts of N₂ dissociate as flow passes through the shock and composite again near the surface. The associative-ionization reaction forms NO⁺ and e and the mass fractions of them are much less than other species.

After the consideration of aerodynamic heating to the structure, the stagnation temperature rises from 220 K to approximately 2600 K as shown in Figure 3. The ablation of thermal protection material occurs during the heating process and the ablation degradation rate of ablation wall is given in Figure 4. Within the first four minutes, the ablation degradation rate is basically zero and controlled by weak oxidation reactions. During the fourth to tenth minutes, the ablation degradation rate near the stagnation point increased rapidly, indicating that the strong oxidation reactions occur. In the last ten minutes, the ablation degradation rate increases slowly and the ablation process is controlled by sublimation reactions.
The ablation plasma flow field at 20 min is further analyzed and the species mass fraction distribution along the stagnation line is given in Figure 5 and Figure 6. Note that nearly all O are used to form CO rather than NO and NO+. Meanwhile, parts of N form CN with C. The mass fraction of CO near the stagnation point is much larger than other ablation products. The mass fraction distribution of the other air species changed little compared with the non-ablation state.

The pressure and temperature distributions along stagnation point line of initial time versus 20 min are shown in Figure 7 and Figure 8. Ablation effect makes the shock detachment distance increase and affects the pressure and temperature distribution of flow field. Meanwhile, the peak temperature near stagnation point in ablation flow field is lower than that in the non-ablation state, due to the absorption of heat by chemical reactions between ablation products and air after shock wave.

6. Conclusions
In this paper, a numerical approach was developed to study the thermochemical nonequilibrium flow field of a hypersonic hemispherical nose with carbon-based thermal protection material ablation. The ablation flow field was simulated by using a full N-S approach coupled with the heat conduction in structure temperature field. The ablation reaction model was developed based on material oxidation and sublimation process.

Under the condition tested, the ablation of thermal protection material was obvious, resulting in the change of chemical species in flow field. In oxidation process, the ablation reactions consumed much of O in nose regions and the primary product was CO. With the increase of surface temperature, sublimation products appeared in the flow field. It was noted that ablation had significant effects on thermochemical nonequilibrium flow. The ablation completely consumed O surrounding the
stagnation point and changed species distribution. Besides, carbon-based material ablation influenced macroscopic flow parameters including shock wave position, pressure and temperature.

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