Numerical Simulation for Hypersonic Flow with High Temperature Thermochemical Nonequilibrium Effect

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Abstract. Numerical simulations were conducted for calorically perfect gas and high temperature thermochemical nonequilibrium gas by CFD methods. Hypersonic Flow with High Temperature Thermochemical Nonequilibrium Effect was studied. The results showed that high temperature effects change the flow field and reduce heat transfer observably. For high temperature flow the kinetic energy associated with hypervelocity flight is converted into increasing the temperature of the air and endothermic reactions including dissociation and ionization of the air past shock. Thus, temperature in the shock layer dramatically decreases. All these works build foundations for further hypersonic aerodynamical computations and engineering applications.

1. Introduction
As hypersonic vehicles fly through the atmosphere, the kinetic energy associated with high velocity is converted into increasing the temperature of the air and into endothermic reactions (as shown in Figure 1), such as dissociation and ionization of the air near the vehicle surface, which is called “high temperature effects” or “real gas effect”. High temperature causes “thermal barrier” and “black barrier” problems which will bring a great impact on the aircraft, as shown in Figure 2. Thus, we must accurately predict thermal environment and provide guidance and reference for thermal protection[1].

![Figure 1. Physical effects characteristic of high altitude and hypersonic flow](image1.png)

![Figure 2. Schematic of thermal barrier and black barrier](image2.png)
The problems associated with determining the aerothermodynamic environment of a vehicle flying through the atmosphere offer challenges to the designer. In general, there are three research methods which include experiment, theory analysis and numerical simulation. The wind tunnel with ground experimental facilities can hardly reproduce the real gas environments which encounters in hypersonic flows. Theory analysis can only give the qualitative conclusion. Numerical simulation is the valuable research means, which gives satisfactory result in most cases.

The aerodynamic heating on aircraft’s surface, which is very serious in flight, has become a remarkable problem for the development of hypersonic vehicles. Aerodynamic heat and force must be predicted to estimate the flight. CFD (Computational Fluid Dynamics) is used to compute the aerodynamical data. The computation of aerothermal flowfield requires the simultaneous solution of the continuity equation, of the momentum equation, and of the energy equation, which is known as Navier-Stokes equations.

The present article is about research of numerical simulation methods and hypersonic aerothermal computations. Numerical methods were conducted for calorically perfect gas and high temperature thermochemical nonequilibrium gas. Hypersonic Flow with High Temperature Thermochemical Nonequilibrium Effect was studied.

2. CFD numerical Methods
Hypersonic aerothermal simulation method for high temperature thermochemical nonequilibrium flow is developed. The reacting Navier-Stokes equations including Park’s two temperature model, Gupta’s air multi-species reaction model and vibrational relaxation were solved to compute aerothermal load. Chemical and vibrational source terms are calculated implicitly which diminishes the stiffness of the calculation, accelerates the calculation’s convergence. The LU-SGS numerical method with source terms was deduced to do the hypersonic aerothermal computation in thermochemical nonequilibrium flow which improves the calculation’s efficiency [2-3].

2.1. 3D N-S equations
The full three dimensional Navier-Stokes equations for hypersonic viscous air flow in thermochemical non-equilibrium are described as following:

\[
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} - (\frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + \frac{\partial G_v}{\partial z}) = S \tag{1}
\]

\[
Q = \begin{bmatrix}
\rho \\
\vdots \\
\rho_{ns} \\
\rho_u \\
\rho_v \\
\rho w \\
\rho E \\
\rho_{ve} \\
\end{bmatrix}, \quad E = \begin{bmatrix}
\rho u \\
\vdots \\
\rho_{ns} u \\
\rho u v \\
\rho v^2 + p \\
\rho w v \\
\rho w E \\
\rho_{ve} u \\
\end{bmatrix}, \quad F = \begin{bmatrix}
\rho v \\
\vdots \\
\rho_{ns} v \\
\rho v u \\
\rho v^2 + p \\
\rho v w \\
\rho v E \\
\rho_{ve} v \\
\end{bmatrix}, \quad G = \begin{bmatrix}
\rho w \\
\vdots \\
\rho_{ns} w \\
\rho w u \\
\rho w v \\
\rho w w \\
\rho w E \\
\rho_{ve} w \\
\end{bmatrix}, \quad S = \begin{bmatrix}
\dot{\omega}_1 \\
\vdots \\
\dot{\omega}_{ns} \\
\dot{\omega}_{ve} \\
\end{bmatrix} \tag{2}
\]

The vector \(Q\) is conservative variables, \(E, F, G\) are the inviscid flux vector, \(E_v, F_v, G_v\) are the viscous flux vector, and \(S\) is the source term. \(i=1, \ldots, \text{ns}\), \(\text{ns}\) is the total number of species in gas mixture.

2.2. Thermodynamics models
The thermal model used here takes into account translation-rotational temperature and vibrational temperature. The internal energy of mixture per unit mass includes the translational, rotational contributions.
\[ e = \sum_{i=1}^{ns} Y_i e_i, \quad e_i = e_{r}^{i} + e_{rot}^{i} + e_{vib}^{i} + e_{el}^{i} + e_{0}^{i} \]  
\[ h = \sum_{i=1}^{ns} Y_i h_i, \quad h_i = \int_{T_0}^{T} c_{p,i} dT + h_0^{i} \]

Where \( h_0^{i} \) is the chemical enthalpy per unit species \( i \). \( c_{p,i} \) is the specific heat at constant pressure of species \( i \).

### 2.3. Multi-species Chemical Reaction Models

An eleven species air model \( (+++, +++, +++, +++, +++, +++, +++, +++, +++, +++, +++, +++, +++, +++, +++, +++, +++, +, +++) \) is implemented to account for the chemical reactions. The reaction is governed by forward and backward reaction rate coefficients \( k_{f,j}, k_{b,j} \) which are evaluated by means of the Arrhenius formulas. The finite rate chemical reaction models are shown as following equation:

\[ \sum_{j=1}^{nr} v_{j}C_{j} \Leftrightarrow \sum_{j=1}^{ns} v_{f,j}C_{j}, \quad j=1, 2, ..., nr \]

### 3. Computation and Analysis

#### 3.1. Computation Conditions

The computational condition comes from reference [4], one of flow condition is used as the 2D cylinder test case which had experiment data for comparison. Flow condition is given in Table.1.

| Freestream conditions | Component conditions |
|-----------------------|----------------------|
| \( Ma \)              | \( 8.78 \)            | \( Y_O \)          | \( 0.07955 \) |
| \( p_\infty \) (Pa)   | \( 687 \)             | \( Y_N \)          | \( 1.0E-9 \) |
| \( T_\infty \) (K)    | \( 694 \)             | \( Y_{O_2} \)      | \( 0.1340 \) |
| \( u_\infty \) (m/s)  | \( 4776 \)            | \( Y_{N_2} \)      | \( 0.73555 \) |
| \( \rho_\infty \) (kg/m\(^3\)) | \( 0.00326 \)       | \( Y_{NO} \)      | \( 0.0509 \) |

Figure 3. Schematic of HEG wind tunnel(left) and cylinder(right)

#### 3.2. Computational Mesh

The CFD grid and discretization of the computational domain are shown in Figure 4.
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Figure 4. Computational mesh

The discretization of the computational domain is shown in Figure 4. Due to its symmetry and computational cost, half domain was adopted to simulate the hypersonic flow. In order to capture boundary layer flow and wall heat transfer, grid refinement was performed in the normal direction. Grid convergence was conducted, and the first grid distance was set to $2.0 \times 10^{-5}$, which ensures the Cell Reynolds Numbers $Re_{\triangle} < 10$.

3.3. Results and Analysis

Using above methods, grid and flow condition, hypersonic aerodynamical simulation was conducted both for high temperature thermochemical nonequilibrium flow and calorically perfect gas flow.

Pressure, density and temperature contour comparison between calorically perfect gas flow and high temperature thermochemical nonequilibrium flow are shown in Figure 5. The detached distance of bow shock reduced significantly for non-equilibrium gas model, the density past shock was significantly greater than the perfect gas, while the temperature past shock is less than the perfect gas. These were due to vibration excitation, dissociation and ionization in the shock layer. The temperature vibrational temperature, $N_2^+$ and $e^-$ mass fraction contour was shown in Figure 6, which is the evidence of above reactions.

The pressure behind shock is higher considering high temperature effects. Real gas effects are expected to affect stability and control derivatives of vehicle, in particular its pitching moment, as highlighted by first U.S Space Shuttle re-entry (STS-1) where an unexpected higher nose-up pitching moment required a body-flap deflection twice the one predicted by the pre-flight analyses to trim the Orbiter \cite{5}.
Nondimensional density and temperature data along the stagnation line were listed in Figure 7 and Figure 8. In this case $Ma_{\infty} = 8.78$, $\frac{\rho_2}{\rho_1} \Big|_{\gamma=1.4} \approx 5.635$ as estimated by normal shock theory with calorically perfect gas. While in high temperature gas model, the $\frac{\rho_2}{\rho_1}$ is much larger than that in calorically perfect gas condition, which causes the shock layer thinner. As to the temperature, $\frac{T_2}{T_1} \approx 15.9$ which means $T_2$ reach 11034.6K. But $T_2$ is only about 7634K, due to the above endothermic reaction.

In order to verify the accuracy of the algorithm, the computational results are compared with the experimental data. In Figure 9, the numerical simulation flow field structure is consistent with wind tunnel schlieren photo, which shows the detached distance of shock matched very well. Heat transfer and pressure distribution along the wall was shown in Figure 10 and Figure 11. As one can see, numerical data (current and reference [4]) and experimental data compare very well, thus confirming that the current CFD method gave a reliable result and could be used to further engineering application.
4. Conclusion

Real gas effect is very important for hypersonic vehicles and Re-entry aircrafts. The air couldn’t be considered as calorically perfect gas due to a series of physical and chemical reactions. All these reactions would influence the aerodynamical and thermal loads of the aerocrafts. In order to investigate the phenomena and mechanisms, numerical simulation methods for high temperature thermochemical nonequilibrium gas were developed. High temperature effects were computed and researched in hypersonic flow.

The detached distance of bow shock reduced significantly for non-equilibrium gas model, the density past shock was significantly greater than the perfect gas, while the temperature past shock is less than the perfect gas. These were due to vibration excitation, dissociation and ionization in the shock layer. It’s proved that the real gas effects are important which can influence the aerodynamic and aerothermal loads. The computational flowfield, heat flux and pressure along the wall surface is compared to experimental data, which proves that current methods are accurate and reliable.

The methods and computations would be applied to future engineering research.

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