HIGH-TEMPERATURE IONIZED AIR RADIATION SIMULATION ON UNSTRUCTURED GRIDS

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Abstract

A numerical method which is based on unstructured grids to compute high-temperature ionized air radiation is described. The multi-species N-S equations are used and the chemical model includes 11 species (O_2,N_2,O,N,NO, NO^+ , N^+,O^+,N^+_2 , O^+_2 , e^-) and 20 reactions. For simulating thermal non-equilibrium effect, the two-temperature model is considered. The finite volume method (FVM) is used for spatial and directional discretization for the RTE on unstructured grids. The code can deal with different kinds of species and radiative bands. Particularly, the Delta, Epsilon, Beta prime and Gamma prime bands of NO are considered in this paper. The numerical results of MUSES-C for hypersonic flow with high-temperature ionized radiation are shown, and compared well with the reference data and experimental data.

1 Introduction

When a reentry capsule crosses the atmosphere at a very high speed, the temperature around it may become sufficiently high to emit a significant amount of radiation. The radiation emanates mainly from the regions of the shock layer where the flow is highly or almost totally dissociated and significantly ionized. When the radiation passes through the cold boundary which is near the wall, the radiation is absorbed by the air, so the boundary is heated. That is to say, the region around shock wave is cooled. When the magnitudes of the involved radiation are as large as the convective heat flux at the wall, the radiation must be considered in the calculation of the heat load to the vehicle. To solve this problem, there already exist some famous programs[1,2,3] such as NONEQ, etc. But most of them only are applied to the structured grids. The numerical approaches with unstructured grids for computation of radiative heat transfer still not go far. The unstructured methods have received little attention on radiative heat transfer for the hypersonic flows, and a few studies have been found only very recently. Vaidya, Murthy and Mathur[4,5] had presented an unstructured finite volume methodology based on the discrete ordinate formulation to calculate the radiation heat transfer. The results were satisfactorily validated.

The objective of this paper is to obtain an accurate computational method to simulate both the thermal-chemical non-equilibrium and air radiation on the same unstructured grids at high temperature situation. Experimental results are used to validate the numerical results of this paper.

2 The basis of this method

2.1 Governing equations

The conservation form of the governing equations is shown as follows

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{E}}{\partial x}+\frac{\partial \mathbf{F}}{\partial y}+\frac{\partial \mathrm{G}}{\partial z}=\frac{\partial \mathbf{E}_v}{\partial x}+\frac{\partial \mathbf{F}_v}{\partial y}+\frac{\partial \mathrm{G}_v}{\partial z}+\mathbf{S} \qquad (1)$$

The corresponding expressions for the inviscid fluxes E (in the x direction), F (in the y direction) and G (in the z direction), and viscid flux E_v、F_v、G_v are well known, so they will not be written here. The S in the right-hand side of the

equation is the source term. Here, the conserved variable U and the source term are of the form

$$\mathbf{U}=[\rho_1,\cdots,\rho_{ns},\rho u,\rho v,\rho w,e_t,e_v]^T \tag{2}$$

$$\mathbf{S}=[\dot{\omega}_1,\ \cdots,\ \dot{\omega}_{ns},\ 0,\ 0,\ 0,\ Q_r,\dot{\omega}_v]^T \tag{3}$$

The quantities ρ_i denote density of the species i, and e_t ,e_v are the total energy and vibrational energy, respectively. The quantities $\dot{\omega}_i$ are the rate of production of species i by chemical reactions and Q denotes the rate of energy gained by the radiative transport phenomenon (radiative source term).

2.2 Spatial and angular discretization of RTE

The equation of radiative transfer (RTE) can be written as:

$$\frac{dI_\eta}{ds}=-\kappa I_\eta+J \tag{4}$$

Here η denotes radiation direction, the Iη is the intensity in η direction. κ is absorption coefficient. The equation of radiation transfer is discretized using a finite volume method (FVM)[8]. The design of control volumes and control angles needed for the spatial and directional discretization is based on the methodology proposed by Raithby and Chui[7] The spatial domain is divided into a finite number of control volumes (triangular and/or quadrilateral elements for two-dimensional geometries, and tetrahedral, prismatic and/or hexahedral meshes for three-dimensional geometries). Similarly, the directional domain is divided into a finite number of control angles. The control angles proposed by Raithby and Chui are defined by constant spacing in the θ and φ directional coordinates. The integration of Eq. (4) over a control volume element and control angle element leads to the following discretized equation:

$$\sum_{i=1}^{face} D_i^l I_i^l A_i=(-\kappa I_p^l+\kappa I_b)\Delta v_p\Delta\Omega^l \tag{5}$$

Where， $D_i^l=\int_{\Delta\Omega^l}(\hat{n}_i\cdot\hat{s})d\Omega$, $\Delta\Omega^l=\int_{\phi^{l-}}^{\phi^{l+}}\int_{\theta^{l-}}^{\theta^{l+}}\sin\theta\,d\theta\,d\phi$.

In this work, face intensities are related to cell values by using the following method:

$$\mathbf{I}_i^l=\begin{cases}\mathbf{I}_p^l;\mathbf{D}_i^l>\mathbf{0}\ (\textbf{out of cell p})\\ \mathbf{I}_{nb}^l;\mathbf{D}_i^l<\mathbf{0}\ (\textbf{into cell p})\end{cases} \tag{6}$$

Here nb equals to cell sharing face i with cell P.

2.3 Thermal nonequilibrium and Chemical reaction model

To take account of thermal nonequilibrium, we consider two terms to describe the relaxation processes. The two terms are:

$$\dot{\omega}_v=\frac{e_v(T_t)-e_v(T_v)}{\tau_v}+\sum_{i=mol}\dot{\omega}_i\widehat{D}_i \tag{7}$$

The first term is for the relaxation process between translational and vibrational energies. The relaxation time is calculated by using the following expression，

$$\tau_v=\tau_v^{MW}+\tau_v^{P} \tag{8}$$

where τ_v^{MW} is the semi-empirical correlation presented by Millikan and White[9]，

$$\tau_v^{MW}=\frac{\sum_{j\neq e}N_j\exp[A_{sj}(T^{1/3}-0.015\mu_{sj}^{1/4})-18.42]}{\sum_{j\neq e}N_jP} \tag{9}$$

$$\mu_{sj}=\frac{M_sM_j}{M_s+M_j},$$

$$A_{sj}=1.16\times10^{-3}\mu_{sj}^{\frac{1}{2}}\theta_{vs}^{\frac{4}{3}}.$$

τ_v^P is the correction term suggested by Park[10] and is effective for T >8000k, which is defined by

$$\tau_v^p=(\sigma_v\bar{c}_sn_s)^{-1}, \tag{10}$$

where $\bar{c}_s=(\frac{8RT}{\pi M_s})^{\frac{1}{2}}$ are the acoustic speed of species s, ns and σ_v are the total number density of heavy particles, and the cross section of vibrational excitation respectively.

The second term is for the process that certain amount of energy is removed at dissociation or is added at recombination of molecules. The energy lost is commonly assumed to be the average vibrational energy at the local condition $\bar{e}_v$. Because dissociation from a higher vibrational state may be more probable (the concept of preferential

dissociation), the following expression is used in present work.

$$\hat{D}_i = \begin{cases} \bar{e}_v , & Tv < 8000K \\ c_1 \bar{e}_v, & 8000K < Tv < 12000K \\ c_2 D, & Tv > 12000K \end{cases} \quad (11)$$

where $c_1>1$，$0.3>c_2>0.8$，and D is dissociation energy of a molecule measured from its ground state.

For high temperature ionized air there are eleven primary constituents (O_2, N_2, O, N, NO, NO^+, N^+, O^+, N^+_2 , O^+_2 , e^-). The possible reactions between these species are listed Table 1 in the flowing:

The possible reactions between these species are listed in table 1. The chemical reaction rate model is Roop N. Gupta's model. Reaction rates are assumed to be a function of controlling temperature Tf and Tb depending on the type of reaction. The controlling temperatures are shown in Table 1. And the Td in Table 1 is $T_d = \sqrt{T_t T_v}$.

Table 1 chemical reaction model

chemical reaction	Tf	Tb
N2+M2=2N+M2: M2=O,O2,N2,NO	T_d	Tt
O2+M1=2O+M1:M1=O,N,O2,N2,NO	T_d	Tt
N2+N=3N	T_d	Tt
NO+M3=N+O+M3:M3=O,N,O2,N2, NO	T_d	Tt
O+NO=O2+N	Tt	Tt
N2+O=NO+N	Tt	Tt
n+o=(no+) + (e-)	Tt	Tv
o+(e-)=(o+) + (e-)+(e-)	Tv	Tv
N+(e-)=(N+)+(e-)+(e-)	Tv	Tv
O+O=(O2+)+(e-)	Tt	Tv
O+(O2+)=O2+(O+)	Tt	Tt
N2+(N+)=N+(N2+)	Tt	Tt
N+N=(N2+)+(e-)	Tt	Tv
O2+N2=NO+(NO+)+(e-)	Tt	Tv
NO+M4=(NO+)+(e-)+M4	Tt	Tv
O+(NO+)=NO+(O+)	Tt	Tt
N2+(O+)=O+(N2+)	Tt	Tt
N+(NO+)=NO+(N+)	Tt	Tt
O+(NO+)=O2+(N+)	Tt	Tt
O2+(NO+)=NO+O2+	Tt	Tt

2.4 Radiation model and Band model

Emission and absorption of radiation in a gas result from transitions between energy levels. In atomic species, all electronic energy levels as well as free electrons may be involved in radiative transitions. For molecules, radiation also occurs due to transitions between rotational and vibrational energy levels. Atomic radiation arises from bound-bound transitions (atomic lines), bound-free transitions (photoionization or radiative deionization), and free-free transitions (Bremsstrahlung radiation). The atomic line data in the present study takes from NIST's data base. Table 2 list the basic information of the atomic lines used in the study. Molecular radiation is more complex because of the large number of energy levels available for transitions. The resulting structure of closely-spaced lines is referred to as a molecular band system. In present study, 10 bands are considered. The basic information of these bands is listed in Table 3.

Table 2 atom line data

atom	Total line	Total Energy level
N	115	356
N+	73	178
O	91	577
O+	378	275

Table 3 molecular line data

molecule	state	Transition
O2	$B3\Sigma u-$	$B3\Sigma u- \rightarrow X3\Sigma g-$
	$X3\Sigma g-$	s-r
N2	$C3\Pi u$	$B3\Pi g \rightarrow A3\Sigma u+$
	$B3\Pi g$	First positive
	$A3\Sigma u+$	$C3\Pi u \rightarrow B3\Pi g$
		Second positive
NO	$E^2\Sigma^+$	$A2\Sigma+ \rightarrow X^2\Pi r$
	$B'^2\Delta$	γ band
	$D^2\Sigma^+$	$B2\Pi r \rightarrow X^2\Pi r$
	$C^2\Sigma^+$	β band
	$B2\Pi r$	$C^2\Sigma+ \rightarrow X^2\Pi r$
	$A2\Sigma+$	δ band
	$X2\Pi r$	$D^2\Sigma^+ \rightarrow X^2\Pi r$
		ε band
		$B'^2\Delta \rightarrow X^2\Pi r$

		β ′ band
		$E^2\Sigma^+ \rightarrow X^2\Pi$ r
		γ ’ band
N2+	*B2 Σu+*	*B2 Σu+ →X2 Σg+*
	X2 Σg+	First negative

2.5 Numerical method and boundary condition

The numerical method that was used to solve the governing equations is based on Jameson’s finite volume method. The boundary condition is the same as the common solution of thermal nonequilibrium. A nearly converged solution is first obtained neglecting radiation, prior to the radiation-coupled calculation. To increase the efficiency, the Planck’s average absorption coefficient is used during here.

3 Results and discussion

The MESES-C reentry capsule is used as the computational model to validate the above method. In this study we focus on the flight condition at the reentry velocity more than 10km/s. The MUSES-C reentry capsule is part of an asteroid sample return mission and will reenter the Earth’s atmosphere at about 12km/s. The peak heat loading to the vehicle is predicted to be at an altitude of 65km when its velocity is 11.6km/s. At the altitude of 65km, the atmospheric density is 1.645E-4Kg/m^3 and the temperature is 233.25K. The geometry for the MUSES-C reentry capsule is sphere-cone shape with a nose radius of 200mm, a cone angle of 45 degrees and a base diameter of 400 mm.

Figure1 is the computational mesh for this model. In Figure2, the temperature along the stagnation streamline is shown. Figure 3 gives the distribution of species, from this figure we can see that behind the shock wave almost all the molecules dissociate, and some particles ionize. Because of the ionized reaction, many free electrons are produced. And these electrons which are adjacent to the wall lead to the free-free transition and bound-free transition. In order to check the radiation calculation, the emission intensity is calculated and compared with the R156 experiment data[6,7]. In this paper, the Delta, Epsilon, Beta prime and Gamma prime bands of NO were considered. From Figure 4 and Figure 5, we can obviously find that our computational results had excellent agreement in shape and absolute intensity between the experimental and numerical spectra for different bands in the calculation. Also we can get that the spectra ranging from 300 to 450 nm are dominant.

4 Conclusions

An unstructured finite volume method for radiative heat transfer has been presented by this paper. An excellent agreement in shape and absolute intensity is obtained between experimental and numerical spectra. The radiative heat flux environment for the MESES-C reentry capsule which reenters at a superorbital speed is also analyzed.

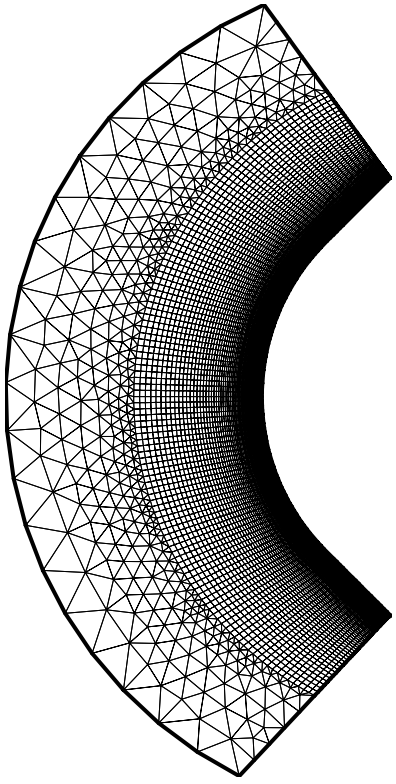

Fig.1 Grids of MESES-C

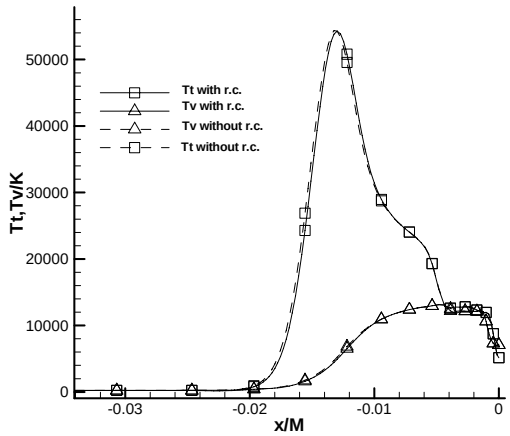

Figure 2. temperature along the stagnation streamline（‘r.c.’ denotes coupling with calculation of radiation）

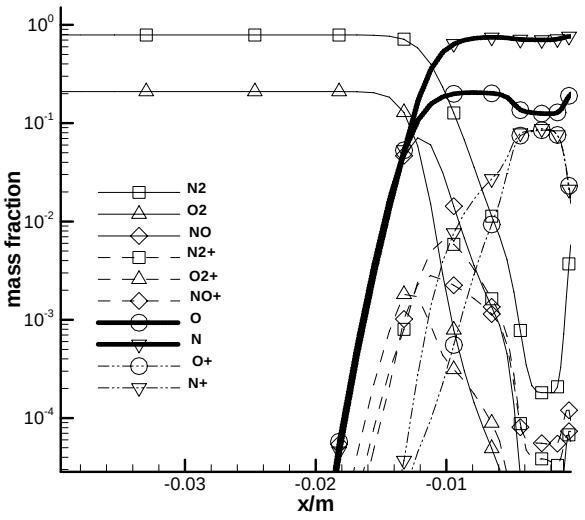

Fig.3 Mass fraction along the stagnation streamline

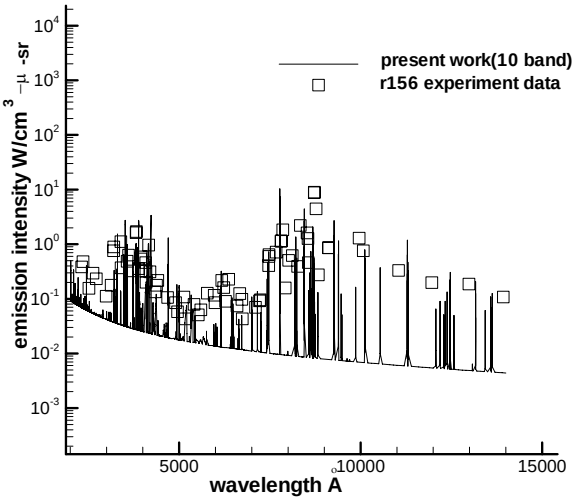

Fig.4 Emission intensity compared with R156 (equilibrium,10 bands)

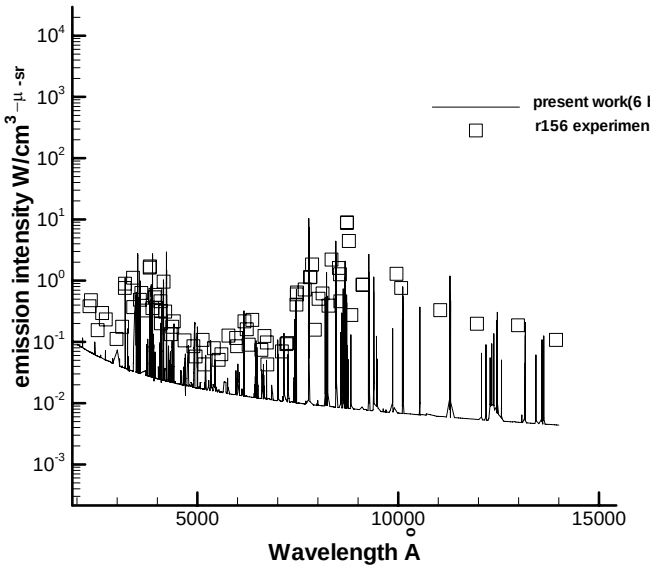

Fig.5 Emission intensity compared with R156 (equilibrium, 6 bands)

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