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Assessment of nonequilibrium air-chemistry models on species formation in hypersonic shock layer

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ABSTRACT

The present study aims to assess the performance of chemical rate models for species formation in the reacting shock layer flows over the blunt-cone hypersonic vehicles. Three 11-species nonequilibrium chemical models for air, Gupta 90, Park 93 and Ozawa's modified models, are assessed. Two controlling temperature expressions ($T^{0.5}T_v^{0.5}$ and $T^{0.7}T_v^{0.3}$) for dissociation reactions are taken into account in these chemical kinetic models. To further examine the performance of these models for predictions of nonequilibrium effects and species formations in the shock layer, two typical flight cases are adopted: (1) the NO formation in reacting flows over the Bow-shock Ultraviolent (BSUV) vehicle at Mach number 17.7, and (2) the electron formation over the Radio Attenuation Measurements (RAM) C-II vehicle at Mach number 23.9 and 25.9. Firstly, comparisons of interested parameters between the computed results in different rate models and available reference data are carried out. Secondly, the reasons for the difference of species formations in these models are discussed. Results show that both the chemical rate model and the weight factor of the controlling temperature have a distinctive influence on species concentration and distribution in the shock layer. The weight factor determines the level of the vibrational-electronic temperature and the reaction release heat in nonequilibrium processes. With the increasing of the weight factor, the NO concentration increases and the electron density decreases in the same rate model. The spectral integration within the wavelengths of 205–255 nm shows that the prediction accuracy of the Park-0.5 and Ozawa-0.7 models is relatively high. Numerical results also indicate that the Ozawa-0.7 model may be an all-round model to predict electron formation in the shock layer.

1. Introduction

Multi-species products play a significant role in the performance of optical detectors installed on the hypersonic vehicle's dome. As all known, the strong shock wave formed in the front of the dome transforms the vehicle's kinetic energy into the internal energy and the temperature of the flows behind the shock rises rapidly. Under such conditions, the chemical kinetic will occur and a large number of neutral particles, free electrons and ions are produced. These products pose many potential problems to the design of hypersonic vehicles. For instance, the nitrogen monoxide (NO) is a critical radiating species in infrared (IR) and ultraviolet (UV) bands, which can result in the strong radiation noise and heating acting on the dome [1,2]. The free electron is also an interested species during flights, which can form a plasma layer around the dome and leads to a loss of communication or "blackout" [3]. Therefore, to accurately predict the reacting flows, especially species formation, is an urgent issue for the design of next generation of hypersonic vehicles.

To simulate the hypersonic reacting flows is a challenge and it involves complex heat and mass transfer problems. For air, a series of chemical kinetics can occur such as exchange, dissociation and ionization when the temperature behind the shock wave reach to several thousand degrees Kelvin. Generally, at above altitudes of 40 km, the time scale of the chemical and internal energy exchange processes are comparable with the characteristic time of flows as the average molecular free path increases [4], meaning flows are thermal and chemical nonequilibrium. To predict such nonequilibrium hypersonic flows, some CFD solvers for have been developed by solving the Navier-Stokes (N-S) equation in the two-temperature (2-T) scheme, such as LAURA [5] and DPLA [6]. In most of CFD codes, several sets of reaction kinetics are used for atmospheric conditions, including Dunn and Kung [7], Park 85 [8], Gupta 90 [9], Park 90 [10] and Park 93 [11]. These rate models are often used for continuum flows. For the high-altitude flows,

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Nomenclature

A	frequency factor, s^{-1} $(m^3/mol)^{n-1}$
a, b	weight factors of the controlling temperature
D_s	diffusion coefficient of the species s, m^2/s
$\hat{D}_s$	average vibrational-electronic energy per unit mass, J/kg
E_a	activation energy, J/mol
H	total enthalpy per unit mass, J/kg
h	enthalpy per unit mass, J/kg
I	Kronecker delta function
$\hat{I}_s$	average translational energy per mole, J/mol
J_s	diffusion flux
k	Boltzmann constant
K_{eq}	equilibrium constant
n	normal derivative on the surface
$n_{f,r}$	temperature exponent
N_d	number of degeneracy states
N_r	number of reactions
p	mixture pressure, Pa
q	heat flux, W/m^2
Re	Reynolds number
t	time, s
T	translation-rotational temperature, K
T_{ve}	vibrational-electronic temperature, K
T_c	controlling temperature, K
$\vec{V}$	mixture average velocity
y_s	mass fraction of species s

Greek symbols

$\dot{\omega}_s$	mass formation rate vector, $kg/(m^3 \cdot s)$
$\dot{\omega}_{ve}$	internal or vibrational energy source term, $J/(m^3 \cdot s)$
ρ	density of mixture gas, kg/m^3
ρ_s	density of species s, kg/m^3
μ	dynamic viscosity coefficient, $N \cdot s/m^2$
η	thermal conductivity, $J/m \cdot s$
υ_{es}	effective collision frequency
$\bar{\tau}$	viscous stress tensor
τ_{ve}	relaxation time, s
θ_{ve}	characteristic vibrational temperature, K

Subscript

ve	vibrational-electronic state
s	species
f	forward reaction
b	backward reaction
∞	free stream condition

Ozawa et al. [12] also developed a chemical kinetic model by modifying the Park's and Bird's models to employ in the TCE (Total collision energy) chemistry for the DSMC simulations. In fact, these reaction probabilities are converted from the rate coefficients expressed in the modified Arrhenius. In most cases, a governing temperature expression with $T^{0.5}T_v^{0.5}$ is used in these reaction models to address the nonequilibrium effect on the dissociation rates, such as DPLR and US3D· but it is an exception to LAURA with $T^{0.7}T_v^{0.3}$ [13]. But up to now, how to select the governing temperature expression in these reaction models is still empirical and is not clear in detail.

In recent years, some progress has been achieved in the comparative studies of different reaction models for earth reentry flows. Hash et al. [13] calculated the aerothermal environments over the FIRE II vehicle with three hypersonic computational fluid dynamics codes of DPLR, LAURA, and US3D. Results showed that different models have at most a 7% difference in convective heating levels. Hao et al. [14] predicted the flows of the RAM-C II and FIRE II vehicles adopting Gupta 90 and Park 90 rate models. Results demonstrated that two models had significant different distributions of ions and electrons and yield distinctively different thermochemical nonequilibrium processes. Surzhikov et al. [15] also stated that the nonequilibrium chemical kinetics model had a greater influence on the radiation by comparing between the Park 93 and the Dunn-Kang model. However, whether the modified Arrhenius rates in the Ozawa's model can be used for continuum flows and how does the controlling temperature affect hypersonic flows are still relatively insufficient in previous studies. Wang et al. [16] assessed the performance of different chemical kinetic models for heat transfer acting on three test cases. It is demonstrated that the difference of heat flux is significant for these rate models, which are more obvious with the increasing of complexity of the vehicle's geometry. To sum up, most of these studies pay more attention to heat transfer in the hypersonic flows for the difference of chemical kinetic models. Obviously, carrying further the investigation into species formation in hypersonic reacting flows are still relatively insufficient in previous studies.

In the present study, three nonequilibrium finite-rate models including Gupta 90, Park 93 and Ozawa's modified models and two governing temperature expressions ($T^{0.5}T_v^{0.5}$ and $T^{0.7}T_v^{0.3}$) will be adopted to simulate the hypersonic reacting flows. Firstly, two typical cases, the BSUV and RAM-C II flight experiments, are employed to examine the species formations of NO and electron, respectively. Then, analysis of chemical rate coefficients for these two species are performed. The effects of both the reaction rate model and the weight factor in the controlling temperature on species formation in the shock-layer flows have been brought out clearly.

2. Numerical models

2.1. Fluid governing equation

For multi-species hypersonic reacting flows, the real gas effect should be employed by the solving the Navier-Stokes (N-S) equations with thermal-chemical nonequilibrium processes. The basic physical principles of conservation of mass, momentum and energy can be written as [17]:

The continuity equation is:

$$\frac{\partial \rho y_s}{\partial t} + \nabla \cdot (\rho \vec{V} y_s) + \nabla \cdot J_s = \dot{\omega}_s \tag{1}$$

where ρ is the mixture density, t is the time, and $\vec{V}$ represents the mixture average velocity. y_s is the mass fraction of species s, and J_s denotes the diffusion flux. $\dot{\omega}_s$ is the net rate of production of species s due to the chemical reactions.

The momentum conservation equation is:

$$\frac{\partial \rho \vec{V}}{\partial t} + \nabla \cdot (\rho \vec{V} \vec{V}) + \nabla p = \nabla \cdot \bar{\tau} \tag{2}$$

where p is the mixture pressure. $\bar{\tau}$ is the viscous stress tensor. According to rigorous kinetic theory, the stress tensor contains two the viscosity coefficients, namely the shear viscosity coefficient