Numerical investigation of oxygen thermochemical nonequilibrium on high-enthalpy double-cone flows

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ABSTRACT

Hypersonic thermochemical nonequilibrium flows over a double-cone configuration are numerically investigated. Simulations with oxygen as the test gas are performed using different coupling models of vibrational excitation and dissociation, including a conventional two-temperature model as the baseline and an improved model established on elementary kinetics and validated against existing shock tube experimental data. For the condition with the highest total enthalpy, the improved model predicts a larger separation region and greater peak heat flux with relative differences of 20.3% and 29.2%, respectively, compared with the baseline two-temperature model. The differences are attributed to inaccurate modeling of the vibration–dissociation coupling effects by the conventional two-temperature model, which overestimates the post-shock degree of dissociation and underestimates the post-shock temperature. The size of the separation bubble is therefore altered due to the change in its density. These findings may help to explain the large discrepancies found between numerical results and experimental data for high-enthalpy double-cone flows in hypersonic studies.

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1. Introduction

Over the past several decades, hypersonic flight technology has attracted growing interest in both the military and non-military communities [1]. The continuous advances in hypersonic systems require a deep understanding of the flow characteristics over these vehicles. An important flow phenomenon that occurs in hypersonic flights is shock-wave/boundary-layer interaction (SWBLI), which can lead to a loss of control authority, peaks in surface heat transfer, and an adverse structural response induced by unsteadiness [2].

SWBLI can be effectively studied with various canonical configurations, including compression corners, shock impingement on flat plates, double wedges, and double cones. Among these models, the axisymmetric double-cone configuration is regarded as an important building block to understand SWBLI in hypersonic flows, which is able to sustain a strong interaction phenomenon, yet obviates the three-dimensional effects induced by the side walls in the two-dimensional counterparts [2,3].

Experimentally, hypersonic flow over a double cone has been systematically investigated at Calspan—University of Buffalo Research Center [4–9]. From 2001 to 2010, a series of double-cone experiments was conducted in the LENS I reflected shock tunnel with total enthalpies ranging from 3 to 15 MJ/kg in air, nitrogen, and oxygen. It was later found that the vibrational and chemical nonequilibrium in the freestream of the LENS I tunnel could have significant effects on the shock standoff distance and surface heating [8,10]. Therefore, in 2013, Holden et al. [9] conducted a new set of experiments in the LENS XX expansion tunnel, which provided a clean freestream environment without frozen vibrational energy and chemical compositions, with total enthalpies ranging from 5 to 22 MJ/kg in air.

The two sets of double-cone experiments have been widely used for computational fluid dynamics (CFD) code validation. Numerical simulations that correspond to the first set were presented by Candler et al. [11], Gaitonde et al. [12], Nompelis et al. [13], Druguet et al. [14,15], and Knight et al. [16]. These studies found that good agreement with experimental measurements could be obtained for the nitrogen flow cases without obvious dissociation, whereas large discrepancies were observed for the air and oxygen flows in the presence of thermochemical nonequilibrium. It was therefore suspected that the vibrational and chemical nonequilibrium in the freestream of the LENS I tunnel and the inaccurate modeling of oxygen vibrational excitation and dissociation could be responsible for the discrepancies [9]. However, although a clean freestream was provided in the LENS XX tunnel, discrepancies were still found between CFD results and the experimental

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Nomenclature

e	specific total energy, J/kg		Q_v	vibrational partition function
e_v	specific vibrational energy, J/kg		$q_{tr,x}$	translational–rotational heat flux in the x direction, J/m²/s
$\mathbf{F}, \mathbf{G}$	vectors of inviscid fluxes in the x and y directions		$q_{v,x}$	vibrational heat flux in the x direction, J/m²/s
$\mathbf{F}_v, \mathbf{G}_v$	vectors of viscous fluxes in the x and y directions		T_{tr}	translational–rotational temperature, K
h_s	specific enthalpy of species s, J/kg		T_{ve}	vibrational–electronic temperature, K
$J_{i,x}$	mass diffusion flux of species i in the x direction, kg/m²/s		T_v	vibrational temperature, K
$K_{eq,r}$	equilibrium constant of reaction r, units in cgs		u, v	velocities in the x and y directions, m/s
k_B	Boltzmann constant, 1.3807×10^{-23} J/K		Z	nonequilibrium factor
$k_{f,r}, k_{b,r}$	forward and backward reaction rate coefficient of reaction r, units in cgs		$\alpha_{r,i}, \beta_{r,i}$	stoichiometric coefficients of reaction r
$k_{f,eq,r}$	equilibrium forward reaction rate coefficient of reaction r, units in cgs		ε_i	vibrational energy of molecular oxygen at the i-th vibrational quantum state, J
$k_{V-V-T}(i,j \rightarrow l,m)$, $k_{V-T}(i \rightarrow j)$ forward rate coefficients for vibration–vibration–translation and vibration–translation transitions of molecular oxygen			$\theta_{v,s}$	characteristic vibrational temperature of species s, K
			$\theta_{d,s}$	dissociation temperature of species s, K
$k_{V-D}(i \rightarrow c), k_{V-D}(c \rightarrow i)$ dissociation and recombination rate coefficients of molecular oxygen at the i-th vibrational quantum state, units in cgs			ρ_i	density of species i, kg/m³
			ω_i	mass production rate of species i per unit volume, kg/m³/s
M_i	molecular mass of species i, g/mol		ω_v	source term in vibrational energy equation, J/m³/s
n_s	number density of species s, cm⁻³		ω_{tv}	energy transport between the translational and vibrational modes, J/m³/s
p	pressure, Pa		ω_{vd}	added or removed average vibrational energy due to recombination and dissociation, J/m³/s

data [17]. A more recent study [18] numerically simulated the double-cone flows under conditions corresponding to the recent experiments using two different vibration–dissociation coupling models, including the popular Park model [19] and the coupled vibration-dissociation-vibration (CVDV) model [20]. It was found that the difference between the results from the Park and CVDV models increased with the total enthalpy. Although the CVDV model predicted closer agreement with the experimental data, but the sizes of the separation regions were still significantly underestimated. It was suggested that state-specific simulations should be performed to exclude the inherent defect of the current vibration–dissociation coupling models. However, tracing the temporal and spatial variation of each vibrational level would require considerable computational resources. Consequently, detailed state-specific simulations have been applied only to one- and two-dimensional inviscid flows [21,22]. Calculations of complex viscous flows such as those around a double-cone configuration using the state-specific method with detailed elementary processes have yet to be made.

It is therefore the objective of this study to develop a computationally affordable model for the process of oxygen vibrational excitation and dissociation and to investigate its effects on high-enthalpy double-cone flows in comparison with a conventional two-temperature model. Efforts are devoted to reveal the cause of the great discrepancies found between numerical results and experimental data for such flows. An oxygen vibration–dissociation coupling model is firstly established based on the kinetic rates for elementary processes and validated against existing shock tube experimental data. High-enthalpy double-cone flows are then simulated with the baseline and improved models. Finally, the conclusions are summarized.

2. Governing equations and numerical methods

Under the two-temperature assumption, the translational–rotational energy mode is considered to be fully excited in terms of a translational–rotational temperature T_{tr}, and the vibrational energy of molecules and the electronic excitation energy are in equilibrium corresponding to a vibrational–electronic temperature

T_{ve}. Because only the ground electronic energy level is considered for the species involved in this investigation, T_{ve} is reduced to a vibrational temperature T_v. For axisymmetric flows, the conservation equations of species mass, mixture momentum, total energy, and vibrational energy can be written as follows:

$$\frac{\partial}{\partial t} \int_\Omega \mathbf{U} d\Omega + \oint_{\partial\Omega} [(\mathbf{F} - \mathbf{F}_v)n_x + (\mathbf{G} - \mathbf{G}_v)n_y] y dS$$
$$= \int_\Omega (\mathbf{S} + \mathbf{S}_{axis}) d\Omega, \tag{1}$$

where x and y are the coordinates in the axial and radial directions, respectively. The vectors of the conservative variables and source terms are given by

$$\mathbf{U} = \begin{pmatrix} \rho_i \\ \rho u \\ \rho v \\ \rho e \\ \rho e_v \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} \omega_i \\ 0 \\ 0 \\ 0 \\ \omega_v \end{pmatrix}, \quad \mathbf{S}_{axis} = \frac{1}{y} \begin{pmatrix} 0 \\ 0 \\ p - \tau_{yy} \\ 0 \\ 0 \end{pmatrix}, \tag{2}$$

where ρ_i is the density of species i, ρ is the density of the mixture, u and v are the velocities in the axial and radial directions, respectively, p is the pressure, e is the specific total energy of the mixture, e_v is the specific vibrational energy of the mixture, and ω_i and ω_v represent the production rates of species mass and vibrational energy per unit volume, respectively.

The vectors of inviscid and viscous fluxes in the axial direction are expressed as

$$\mathbf{F} = \begin{pmatrix} \rho_i u \\ \rho u^2 + p \\ \rho u v \\ (\rho e + p)u \\ \rho e_v u \end{pmatrix}, \quad \mathbf{F}_v = \begin{pmatrix} -J_{i,x} \\ \tau_{xx} \\ \tau_{xy} \\ u\tau_{xx} + v\tau_{xy} - (q_{tr,x} + q_{v,x}) - \sum_{s=1}^{ns} J_{s,x} h_s \\ -q_{v,x} - \sum_{s=mol.} J_{s,x} e_{v,s} \end{pmatrix}, \tag{3}$$