



Effects of vibrational nonequilibrium on hypersonic shock-wave/laminar boundary-layer interactions

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ABSTRACT

Recent numerical simulations of hypersonic double-cone and hollow-cylinder flare experiments have incorrectly predicted the sizes of separation regions, even at total enthalpies as low as 5.44 and 5.07 MJ/kg. This study investigates the effects of vibrational nonequilibrium to explain these discrepancies. According to an assessment of various flow models under post-shock conditions in comparison with state-specific simulations, the predictions obtained by treating the vibrational modes of molecular nitrogen and oxygen as a single mode, a strategy adopted routinely by the aerospace computational fluid dynamics community, are in close agreement with the state-specific results in terms of post-shock temperature and density profiles, whereas separation of the vibrational modes and assumption of calorically perfect gases would lead to evident errors. The double-cone flow is found to be sensitive to different flow models. In contrast, their effects on hollow-cylinder flare flow are insignificant. Given that the most representative flow model still underestimates the sizes of the separation regions for double cone flow and overestimates those for hollow-cylinder flare flow, it is concluded that inaccurate modeling of vibrational nonequilibrium may not be responsible for the discrepancies observed at the lowest total enthalpies. Suggestions for further study are also presented.

1. Introduction

Shock-wave/boundary-layer interaction (SWBLI) is frequently encountered in hypersonic flight and can lead to high aerothermodynamic loads. Accurate predictions of SWBLI are of vital importance to the design of hypersonic vehicles.

Extensive experiments [1–6] using canonical configurations have been conducted to evaluate the ability of modern computational fluid dynamics (CFD) tools to predict hypersonic laminar interactions in thermochemical nonequilibrium states. This study investigates the double-cone and hollow-cylinder flare experiments performed in 2013 by Holden et al. [7] in the LENS XX expansion tunnel at Calspan—University of Buffalo Research Center. In these experimental studies, surface pressure and heat flux were measured in air at total enthalpies between 5.44 and 21.77 MJ/kg for a 25–55 deg. double-cone configuration and from 5.07 to 21.85 MJ/kg for a 30 deg. hollow-cylinder flare. The numerical results from various studies [8–14] have been compared with the experimental data. It was found that the CFD simulations tended to underestimate the sizes of the separation regions for the double cone and overestimate the sizes of the separation bubbles for the hollow-cylinder flare. The causes for these discrepancies remain poorly understood. It is commonly suspected that inaccurate modeling

of air chemistry might be a major reason [7]. However, given that very few chemical reactions would occur at the lowest total enthalpies, it may be inferred that the discrepancies observed under these conditions have a different cause. Specifically, this study investigated the effects of vibrational nonequilibrium on the double-cone and hollow-cylinder flare flows at total enthalpies of 5.44 and 5.07 MJ/kg to explain the discrepancies.

The paper is organized as follows: Different flow models are discussed in Section 2, including a mixture of perfect gases with vibrational nonequilibrium, a mixture of perfect gases with vibrational nonequilibrium of separate modes, and a mixture of calorically perfect gases. Section 3 presents an assessment of these models under post-shock conditions using state-specific results as a reference. In Section 4, the distributions of surface pressure and heat flux predicted by different flow models are compared with the experimental data.

2. Flow models

Based on different treatments of vibrational nonequilibrium, three flow models are considered in this work. In these models, the molecules' rotational energy mode is assumed to be fully excited and in equilibrium with the translational mode of heavy particles in terms of a

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translational–rotational temperature, T_{tr} . The processes of electronic excitation and ionization are neglected.

2.1. Model I: mixture of perfect gases with vibrational nonequilibrium

In model I, the flow is assumed to be in thermal nonequilibrium according to Park's two-temperature model [15], in which the vibrational levels of molecules are described by harmonic oscillators and populated in Boltzmann distributions in terms of a single vibrational temperature, T_v . The finite-rate air chemistry is considered to be frozen. Because only molecular nitrogen and oxygen are present in the experimental freestreams, the fluid medium is described as a two-species (N_2 , O_2) mixture with the mass fractions remaining unchanged throughout the flowfields. The corresponding governing equations comprise the conservation equations of species mass, mixture momentum, total energy, and mixture vibrational energy. Here, only the equation of mixture vibrational energy is presented as

$$\frac{\partial \rho e_v}{\partial t} + \frac{\partial \rho e_v u_j}{\partial x_j} = -\frac{\partial q_{v,j}}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\sum_{s=\text{mol.}} J_{s,j} e_{v,s} \right) + \omega_v \quad (1)$$

where the index mol. denotes molecular species; ρ is the density of the mixture; e_v and $e_{v,s}$ are the specific vibrational energies of the mixture and species s , respectively; q_v is the vibrational heat flux vector; J_s is the mass diffusion flux vector of species s ; and ω_v is the vibrational energy source term, given by

$$\omega_v = \omega_{t-v} + \omega_{v-d} \quad (2)$$

The term ω_{t-v} is the energy transfer between the translational and vibrational modes, which is modeled using the Landau–Teller model [16] and the Millikan–White expression [17] with Park's high-temperature correction [18]. The term ω_{v-d} is the added or removed vibrational energy induced by recombination and dissociation, which here is equal to zero due to the frozen chemistry.

Model I is one of the routine options widely used in the aerospace CFD community to represent the vibrational nonequilibrium processes.

2.2. Model II: mixture of perfect gases with vibrational nonequilibrium of separate modes

In model II, the flow is also assumed to be a two-species mixture without chemical reactions. Instead of modeling the mixture vibrational energy, the vibrational modes of molecular nitrogen and oxygen are treated separately with the corresponding conservation equations given by

$$\frac{\partial \rho_s e_{v,s}}{\partial t} + \frac{\partial \rho_s e_{v,s} u_j}{\partial x_j} = -\frac{\partial q_{v,s,j}}{\partial x_j} - \frac{\partial J_{s,j} e_{v,s}}{\partial x_j} + \omega_{v,s} \quad (3)$$

where $s = N_2$ and O_2 . Because no chemistry is considered in this model, the vibrational energy source term, $\omega_{v,s}$, simply contains two parts: $\omega_{t-v,s}$ and $\omega_{v-v,s}$. The $\omega_{t-v,s}$ term is modeled in the same manner as model I, whereas $\omega_{v-v,s}$, which represents the vibrational energy transfer between different molecules, is expressed in the following form [19]:

$$\omega_{v-v,s} = \sum_{r \neq s} N_{Av} \sigma_{sr} \rho_s \rho_r \sqrt{\frac{8k_B T_{tr}}{\pi \mu_{sr}}} \left(P_{sr} \frac{e_{v,r}}{M_s} - P_{rs} \frac{e_{v,s}}{M_r} \right) \quad (4)$$

where N_{Av} is the Avogadro constant, σ_{sr} is the collision cross section, k_B is the Boltzmann constant, μ_{sr} is the reduced mass, M_s is the molecular mass of species s , and P_{sr} is the probability of vibration–vibration exchange between species s and r . For N_2 – O_2 interactions, the probability is taken from Park and Lee [20].

Model II can be regarded as an upgrade of model I, but its accuracy relies on the modeling of $\omega_{v-v,s}$.

2.3. Model III: mixture of calorically perfect gases

To further examine the effects of vibrational nonequilibrium, model III assumes that the flow is described by a two-species mixture of calorically perfect gases. Here, no vibrational excitation is considered, thus the vibrational energy equation can be removed. The corresponding governing equations are similar to the conventional Navier–Stokes equations for a calorically perfect gas except that the conservation of mass is established for each species.

3. Assessment of different vibrational nonequilibrium models

Because the only difference between models I, II, and III lies in the treatment of vibrational nonequilibrium, it is of interest to investigate which model provides the most accurate description of vibrational excitation before the numerical results and experimental data are compared for hypersonic SWBLI. In this section, these models are therefore assessed under post-shock conditions, using the results obtained from the state-specific simulation as a reference.

3.1. State-specific simulation

The vibrational elementary processes considered in the state-specific simulation contain the vibration–vibration–translation (V – V – T) bound–bound transitions induced by N_2 – N_2 , N_2 – O_2 , and O_2 – O_2 collisions. The resulting master equation for the number density of N_2 at vibrational level i can be expressed as

$$\frac{\partial [N_2(i)]}{\partial t} = \left\{ \frac{\partial [N_2(i)]}{\partial t} \right\}_{V-V-T}^{N_2-N_2} + \left\{ \frac{\partial [N_2(i)]}{\partial t} \right\}_{V-V-T}^{N_2-O_2} \quad (5)$$

$$\begin{aligned} & \left\{ \frac{\partial [N_2(i)]}{\partial t} \right\}_{V-V-T}^{N_2-N_2} \\ &= \sum_m \sum_n \sum_j \{ k_{V-V-T}^{N_2-N_2}(m, n \rightarrow i, j) [N_2(m)] [N_2(n)] \\ & \quad - k_{V-V-T}^{N_2-N_2}(i, j \rightarrow m, n) [N_2(i)] [N_2(j)] \} \end{aligned} \quad (6)$$

$$\begin{aligned} & \left\{ \frac{\partial [N_2(i)]}{\partial t} \right\}_{V-V-T}^{N_2-O_2} \\ &= \sum_m \sum_n \sum_j \{ k_{V-V-T}^{N_2-O_2}(m, n \rightarrow i, j) [N_2(m)] [O_2(n)] \\ & \quad - k_{V-V-T}^{N_2-O_2}(i, j \rightarrow m, n) [N_2(i)] [O_2(j)] \} \end{aligned} \quad (7)$$

where $[A]$ represents the number density of species A , $k_{V-V-T}(i, j \rightarrow m, n)$ is the rate coefficient of V – V – T transitions (with superscripts representing the interaction type), and i, j, m , and n represent the vibrational quantum numbers of the colliding molecules. The master equation for O_2 can be established in a similar manner.

The 61 and 46 vibrational levels given by Lopez and Lino da Silva [21] are considered here for molecular nitrogen and oxygen, respectively, in the ground electronic state. The rate coefficients of V – V – T transitions are calculated based on forced harmonic oscillator theory, whose accuracy was validated by comparison with the results determined by semiclassical trajectory calculations for single-quantum transitions [22, 23] by Lino da Silva et al. [24]. Generally, the forced harmonic oscillator model may provide an alternative solution for V – V – T transition rate coefficients when the quasi-classical trajectory data are unavailable.

In the shock reference frame, the master equations are directly coupled to the one-dimensional compressible flow equations to trace the spatial variation of each vibrational level of N_2 and O_2 behind a normal shock. To reduce the computational cost, the multi-quantum V – V – T transitions with jumps larger than 5 are assumed to be negligible according to the heat bath calculations of Andrienko et al. [25] and the post-shock simulations of Hao et al. [26]. The initial condition

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