Nonequilibrium relaxation in high-temperature gas flows

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Abstract

Numerical simulations are presented of steady-state, hypersonic flows for the prediction of multi-translational and rotational temperatures, and vibrational energy distributions, in order to understand the thermodynamic nonequilibrium phenomena encountered along the trajectory of the hypersonic flowfields of aerospace vehicles. A new gas kinetic, multi-translational temperature model for a monoatomic gas was developed by solving equations derived from the Boltzmann equation with a first-order Chapman–Enskog expansion of an anisotropic velocity distribution function. The nonequilibrium vibrational energy distributions were modeled by the master equation and the population distributions in the quantum energy states of the di-atomic molecule evaluated under multiple-quantum vibrational–translational energy exchanges.

Keywords: High-speed, high-temperature, gas flows; Nonequilibrium relaxation; Multi-translational temperature; Rotational and vibrational energy modes

1. Introduction

The presence of shock waves in high-speed flow of an air mixture presents considerable difficulties for accurate numerical simulation of the flowfield. The shock wave redistributes the high kinetic energy of the oncoming flow into various internal energy modes, which relax relatively slowly, leading to significant chemical and thermal nonequilibrium in the stagnation region. In the gas kinetic description, intermolecular collisions change the translational, rotational, vibrational, and electronic energies of the collision partners. The probabilities or effective cross-sections of these elementary processes differ significantly, giving rise to widely separate relaxation times for the internal modes. Thus it becomes important to account for the rates of relaxation processes to predict the nonequilibrium behavior of these kinds of flows [1,2]. The present study simulates nonequilibrium relaxation in high-speed flows, considering multi-translational and rotational temperature modeling. Vibrational relaxation is examined in the context of a master equation approach.

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2. Model development

The Boltzmann equation expresses the behavior of many-particle kinetic systems in terms of the evolution equation for the single particle gas distribution function. The simplified collision model given by the Bhatnagar–Gross–Krook (BGK) model is formulated as

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{f^{eq} - f}{\tau} \tag{1}$$

where f, the distribution function, gives the number density of molecules at position $\mathbf{x}$ and velocity $\mathbf{u}$ at time t. The left-hand side of the above equation represents the free streaming of molecules in space, and the right-hand side denotes the collision term. If the distribution function f is known, macroscopic variables of the mass, momentum, energy and stress can be obtained by integration over the moments of molecular velocity. In the BGK model, the collision operator involves a simple relaxation to a local equilibrium distribution function f^{eq} with a characteristic time scale τ. With the above kinetic model, the Navier–Stokes equations in mass-averaged velocity form can be derived. With the modification of the particle collision time, the validity of the kinetic model is extended beyond that of the Navier–Stokes equations. An earlier attempt based on this model was

successful for shock structure calculations of the monatomic gas with a single translational temperature [3]. This report presents a methodology for obtaining multi-translational temperatures from the BGK model.

Further, to include the internal energy contribution due to the inelastic collisions in the vibrational energy mode, the mass conservation equation can be written to include the source term, $\dot{\omega}_v$

$$\frac{\partial}{\partial t}(\rho_v) + \nabla \cdot (\rho_v \vec{\mathbf{u}}) = \dot{\omega}_v \quad v = 0,1,\ldots \tag{2}$$

Here, ρ_v denotes the state density in the quantum level v of the vibrational manifold. The mass density of the molecular species is the sum of the corresponding state densities in the vibrational levels:

$$\rho = \sum_{v=0}^{v_{last}} \rho_v \tag{3}$$

In the continuum regime, the Navier–Stokes equations could then be used to simulate a flow in thermal disequilibrium. A microscopic kinetic approach was taken (Eq. 2) by treating the molecule as an harmonic oscillator, calculating the state populations using the master equation.

2.1. Multi-translational and rotational temperature modeling

For a gas with different translational temperatures in the x, y, and z directions, an anisotropic distribution is assumed with equilibrium state prevailing in a given direction, and for a one-dimensional flow, written as:

$$g = \rho(\frac{\lambda_x}{\pi})^{1/2}(\frac{\lambda_y}{\pi})^{1/2}(\frac{\lambda_z}{\pi})^{1/2} \exp[-\lambda_x(u-U)^2 - \lambda_y v^2 - \lambda_z w^2] \tag{4}$$

where ρ is the density, U is the macroscopic velocity in the x-direction, and (u, v, w) the components of the particle velocity in the x, y, and z directions, respectively. The parameter λ is related to the gas temperature, given by $\lambda_x = \mathcal{M}/2kT_x$, $\lambda_y = \mathcal{M}/2kT_y$ and $\lambda_z = \mathcal{M}/2kT_z$. For the monatomic gas we construct a generalized BGK model for the translational non-equilibrium

$$f_t + uf_x = \frac{1}{2}[\frac{g-f}{\tau} + \frac{\bar{g}-f}{\tau}] \tag{5}$$

where f is the real gas distribution function, and g and $\bar{g}$ are the corresponding Maxwellians. Note that the particle collision time τ is related to the local dynamical viscosity μ and pressure p, i.e. $\tau = \mu/p$. We reconstructed the particle collision process. Starting from the gas distribution function f for a monatomic gas, the particle collisions drive f to g and $\bar{g}$, instead of from g to $\bar{g}$ alone. During the course of particle collisions, it is difficult to distinguish the process from f to g or that from f to $\bar{g}$. In terms of the particle collision time for translational nonequilibrium, they can be assumed to be the same. Additional features of the model are discussed in [4].

The numerical method developed in [5] is used to solve Eq. 5. For a finite volume method

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x}\int_0^{\Delta t}(F_{j-1/2}(t) - F_{j+1/2}(t))dt + S_j^n \Delta t \tag{6}$$

where W_j^n is the cell averaged mass, momentum, total energy, and the thermal energy in y and z directions, and $F_{j+1/2}$ represents the corresponding fluxes at a cell interface. Note that Δt is the time step $\Delta t = t^{n+1} - t^n$, and S_j^n is the source term for the thermal energy. The evaluation of the fluxes is based on the gas distribution function f at a cell interface.

The present calculations use a monatomic gas with the atomic weight of argon and a Maxwellian (inverse fourth power) inter-atomic potential ($\mu_{ref} = 2.515 \times 10^{-5} kg/ms$, $T_{ref} = 273K$, and $\omega = 1$). Figure 1 plots the mass density and multi-translational temperatures of Maxwellian gas shock wave for free-stream Mach numbers of 5.0 and compared to existing DSMC results. The temperature is resolved in the components perpendicular (x direction) and parallel (y direction) to the shock wave. The results show a good match between the present continuum model and the DSMC calculations.

Figure 2 shows the density distribution, averaged translational temperature, and the rotational temperature in a Mach 7 nitrogen shock wave. The density and rotational temperature are compared with experimental data of Robben and Talbot [6]. The measured rotational temperature and density are accurately predicted by the present continuum model.

2.2. Energy exchanges in the vibrational manifold

To model the vibrational relaxation process, the conservation Eq. 2 is written for the mass density in quantum level v. The source term $\dot{\omega}_v$ derived from the vibrational master equations includes the relevant energy exchange processes consisting of the vibrational–translational (V–T), vibrational–vibrational (V–V), and dissociation. The kinetics of the particle exchanges among the quantum states are simulated using the vibrational master equation; the population distributions are calculated with [7]:

$$\dot{\omega}_v = \frac{1}{\mathcal{M}}\{\sum_{v'}[k_{VT}(v' \to v)\rho_{e'}\rho - k_{VT}(v \to v')\rho_v\rho] + \tag{7}$$

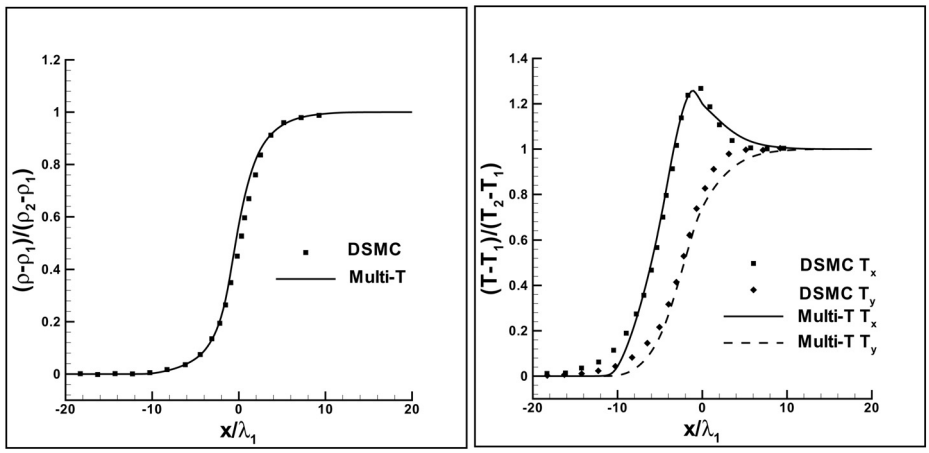

Fig. 1. Computed normalized density and temperatures for a Mach 5.0 Maxwellian gas shock wave.

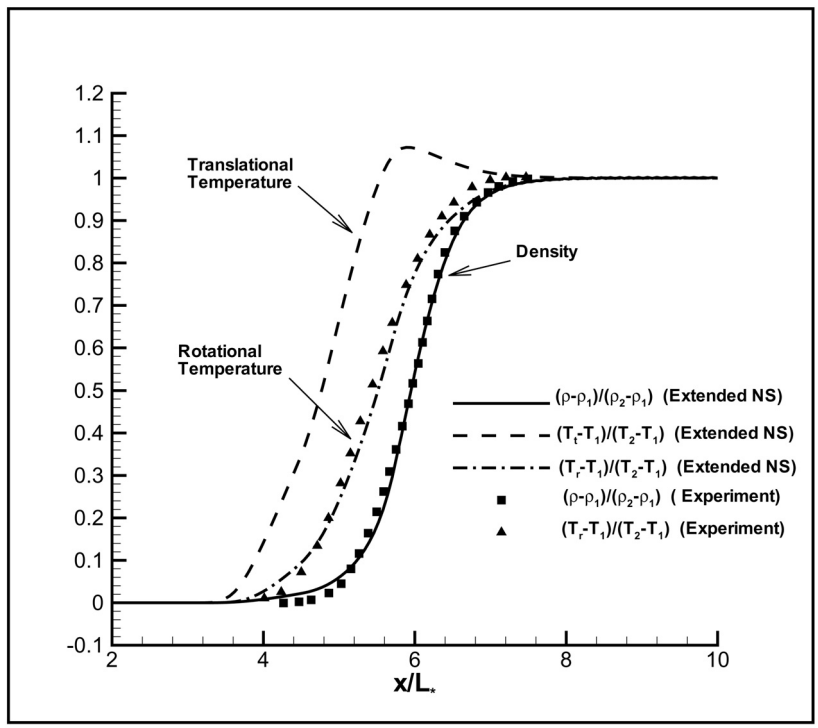

Fig. 2. Computed normalized density and temperatures for a Mach 7 Nitrogen gas shock wave.

$$\sum_{w,v',w'} [r_{VV}(v',w' \to v,w)\rho_{v'}\rho_{w'} - r_{VV}(v,w \to v',w')\rho_v\rho_w]\}$$

The V–T process, shown in the above equations, is associated with the rate coefficient k_{VT} where the molecule loses or gains a vibrational quantum. The de-excitation rate from v' to v is denoted by $k_{VT}(v' \to v)$, and the inverse collision from $v \to v'$ $k_{VT}(v \to v')$. Additional details of the model can be found in [4].

The coupled fluid dynamic equations and the vibrational master equations were solved for a hypersonic flow past a blunt body where the nonequilibrium effects

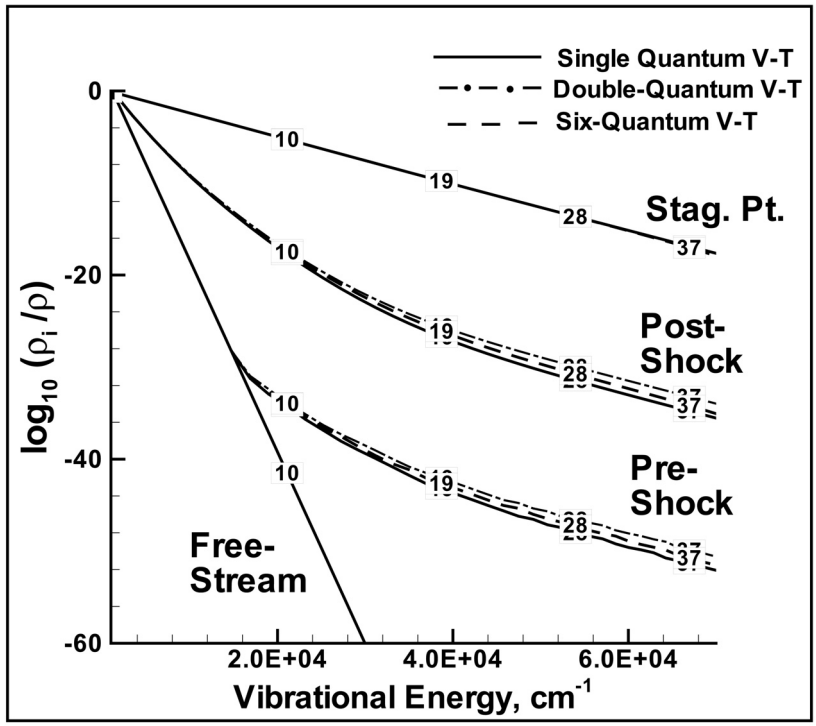

Fig. 3. Population distribution at select locations along stagnation streamline for nitrogen flow past blunt body, r = 1 m, $M_\infty = 6.5$, $T_\infty = 300$ K, $Tv_\infty = 300$ K, $p_\infty = 50$ Pa.

are notable in the vicinity of the shock wave. The flow conditions for the results shown in Fig. 3 are: $M_\infty = 6.5$, $p_\infty = 50$ Pa and $T_\infty = 300$ K, for pure nitrogen flow past an infinite cylinder of 1 meter radius. Figure 3 shows the population distribution for nitrogen along the stagnation streamline at the freestream, pre-shock, post-shock, and stagnation point locations. The deviation of the population distributions from the Boltzmann provides a means of quantifying the nonequilibrium process prevalent in these flows. The negligible influence of multiquantum transitions is also seen in these results.

3. Conclusions

Numerical simulations were performed with a gas kinetic BGK scheme and a Navier–Stokes approach to analyze the translational and internal energy nonequilibrium phenomena that arise in hypersonic aerodynamic flows. A newly developed multi-translational temperature gas kinetic model is based on anisotropy of the molecular velocity distribution function for monoatomic gas shock structures. The present solutions were compared with DSMC solutions. The agreement was excellent. The mass density and rotational temperature predictions for a Mach 7 nitrogen shock structure matched Robben and Talbot's experimental data very well. Detailed flowfield solutions in thermodynamic nonequilibrium were performed where the vibrational master equation was coupled to the fluid dynamic equations. The resulting thermal nonequilibrium of a Mach 6.5 flow past a blunt body was quantified as the deviation from Boltzmann distributions. The results are useful for a better understanding and characterization of the nonequilibrium processes prevalent in hypersonic aerospace vehicle flowfields.

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