

Coupled Hydrodynamic/State-Specific High-Temperature Modeling of Nitrogen Vibrational Excitation and Dissociation

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Vibrational state-specific kinetics are applied to the simulation of high-temperature gas behind strong shocks. A hydrodynamic numerical tool was developed based on recent excitation and dissociation state-resolved models from the FHO theory, and on accurate vibrational energy levels for the N_2 electronic ground-state $X^1\Sigma_g^+$. The master equation is solved in time-dependent, post-shock relaxation and multi-dimensional CFD simulations. The obtained results are compared to classical multi-temperature models often used in the aerospace community for non-equilibrium flow simulations.

There is considerable interest in understanding non-equilibrium processes in shock-heated flows during high-speed atmospheric entries. For very high-temperature conditions, internal level populations significantly depart from the Boltzmann distribution, making the classical multi-temperature models totally in-appropriated. Accurate determination of internal level populations requires the resolution of the so-called master equation, a system of coupled state-specific mass conservation equations associated to each internal level. Rotational levels are assumed to be populated by a Boltzmann distribution at the gas temperature, this assumption being justified by the fast rotational relaxation times. Atomic nitrogen excitation and gas ionisation processes are discarded. Only the electronic ground-state $X^1\Sigma_g^+$ of molecular nitrogen is considered. Its vibrational energy levels are computed through potential-curve reconstruction according to the Rydberg-Klein-Rees method [1]. Solving the corresponding radial Schrödinger equation leads to a total of 61 vibrational bound levels. The FHO theory is used [2] to compute state-specific dissociation and V-T rates, including multiple quantum jumps, for translational temperatures ranging from 100 K to 100 000 K. Reverse reaction rates are calculated using the detailed balance principle. Mass conservation equations associated to all the vibrational levels of $N_2(X^1\Sigma_g^+)$ and to the fundamental level of atomic nitrogen are solved simultaneously along with the total energy and momentum conservation equations, which leads to the following 0D and 1D ODE systems:

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho c_k \\ \rho E \end{bmatrix} = \begin{bmatrix} \dot{\omega}_k \\ 0 \end{bmatrix} \quad \text{and} \quad \frac{\partial}{\partial x} \begin{bmatrix} \rho u c_k \\ \rho u^2 + P \\ \rho u (h + u^2/2) \end{bmatrix} = \begin{bmatrix} \dot{\omega}_k \\ 0 \\ 0 \end{bmatrix} \quad (1)$$

Taking into account both multi-dimensional effects and transport phenomena, the conservative system reads:

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho c_k \\ \rho u \\ \rho v \\ \rho E \end{bmatrix} + \frac{\partial}{\partial x} \left(\begin{bmatrix} \rho u c_k \\ \rho u^2 + P \\ \rho u v \\ \rho u H \end{bmatrix} - \begin{bmatrix} J_{x_k} \\ \tau_{xx} \\ \tau_{xr} \\ \mathbf{V}\tau_x + q_x \end{bmatrix} \right) + \frac{\partial}{\partial r} \left(\begin{bmatrix} \rho v c_k \\ \rho v u \\ \rho v^2 + P \\ \rho v H \end{bmatrix} - \begin{bmatrix} J_{r_k} \\ \tau_{rx} \\ \tau_{rr} \\ \mathbf{V}\tau_r + q_r \end{bmatrix} \right) = \begin{bmatrix} \dot{\omega}_k \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (2)$$

where quantities have their usual notations. In the space relaxation system, post-shock conditions are obtained from Rankine-Hugoniot jump relations assuming frozen gas composition across the shock, upstream internal distributions being boltzmannian. Note that no additional conservation equations are required to describe the vibrational energy time-evolution since this quantity is directly computed from the vibrational levels populations. Considering vibrational excitation and dissociation processes, chemical production rates reduce to:

$$\dot{\omega}_k = M_k \left[\sum_{\mathcal{R}_{Ev}} \left(K_{fi}^{Des} N_{N_2(f)} N_M - K_{if}^{Exc} N_{N_2(i)} N_M \right) + \sum_{\mathcal{R}_{Dv}} \left(K_i^{Rec} N_{N(0)}^2 N_M - K_i^{Dis} N_{N_2(i)} N_M \right) \right]$$

The multi-dimensional case corresponds to a PDE system which is solved using finite volume method. A second-order upwind TVD method based on Harten-Yee discretisation of convective flux is used. Viscous terms are approximated by centred a finite difference scheme, assuming identical transport properties for all internal levels. The low convergence associated with stiff chemical source terms is avoided using an implicit second-order temporal discretisation. The results are compared to multi-temperature simulations based on the usual Landau-Teller model for vibrational relaxation.

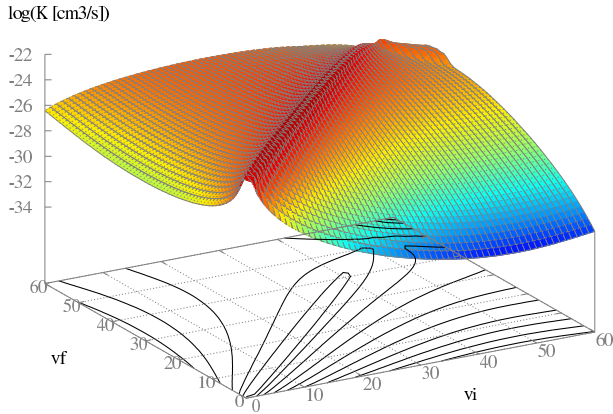


Fig. 2: Multi-quantum V-T reaction rates at 20 000 K for diatomic nitrogen in electronic ground-state $N_2(X^1\Sigma_g^+)$.

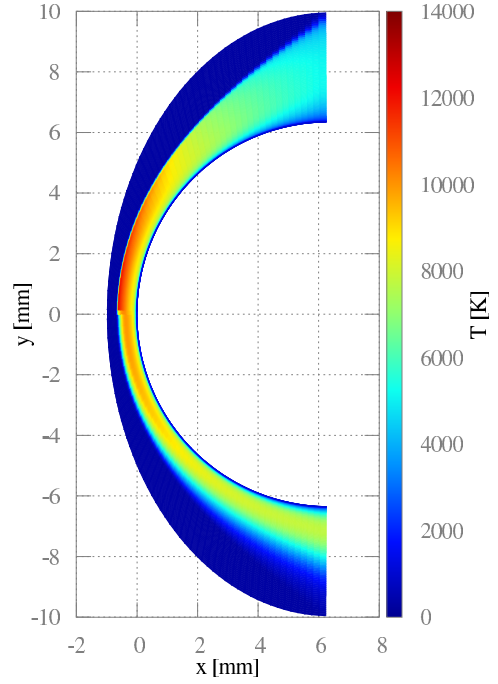


Fig. 1: Distribution of translational (top) and vibrational (bottom) temperatures using a multi-temperature approach.

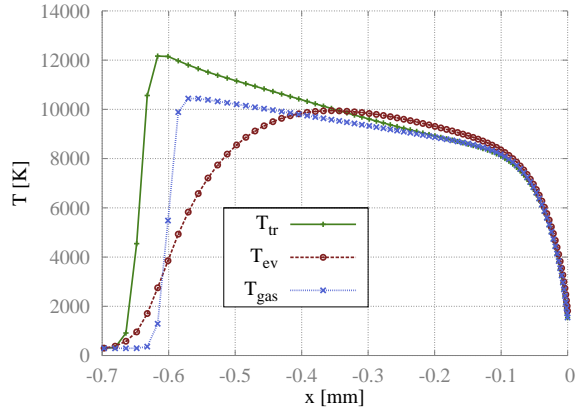


Fig. 3: Translational, vibrational and equilibrium temperatures in a blunt-body shock layer.

- [1] M. Lino da Silva, V. Guerra, J. Loureiro, P.A. Sa, *Vibrational Distribution in N_2 with a Improved Calculation of Energy Levels using the RKR Method*, Chemical Physics **348** (2008) 187-194.
- [2] M. Lino da Silva, V. Guerra, J. Loureiro, P.A. Sa, *State-Resolved Dissociation Rates for Extremely Nonequilibrium Atmospheric Entries*, J. of Thermophysics and Heat Transfer **21** (2007) 40-49.