The Discrete Velocity Method for Solving the Boltzmann Equation with Quantized Internal Energy

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ABSTRACT

A discrete velocity method (DVM) for solving the Boltzmann equation developed at The University of Texas at Austin [1,2,3] has been extended to account for polyatomic molecules with excited internal energy states. A decoupled, quantum description is used for rotational and vibrational energy modes where vibration is described with an anharmonic oscillator and rotation is described with a non-rigid rotor. Removing rotation-vibration coupling terms gives rise to errors, but the difference between the coupled and decoupled models are shown to be within acceptable limits: 1% difference in the partition functions at 3,000 K to 6% difference in the partition functions at 20,000 K for a typical diatomic molecule. Vibrational and rotational distribution functions are stored at every velocity location as independent arrays. The sum over all vibrational levels and the sum over all rotational levels both equal the number density at the velocity location. The initial method models every energy level up to some maximum level number based on the expected maximum temperature. However, such a detailed description has large memory and computational requirements because the total number of values stored at each spatial location is the number of velocity points multiplied by the total number of points used to describe the vibrational and rotational distributions. If each allowed quantum number is used then the total number of points is, $N_{vel}(N_{vib} + N_{rot})$. Because of the computational requirements the full description is limited to simulation of homogeneous relaxation for the purpose of testing and validation of the inelastic collision dynamics. A reduced level number model is developed that decreases the number of simulated levels to be used for flowfield simulations. Quantum states are grouped into a select number of representative levels based on the range of temperatures expected during a simulation, and the entire density grouped at each representative level takes on the energy value corresponding to the level location. Inelastic relaxation rates (Z_v and Z_r), which are measures of the number of elastic collisions compared to the number of inelastic collisions, are accounted for through splitting each depletion into three parts: (1) inelastic collisions with exchanges between vibrational and translational energy for each collision partner and depletion density scaled by $1/Z_v$, (2) inelastic collisions between rotational and translational energy for each collision partner and depletion density scaled by $1/Z_r$, and (3) an elastic collision with depletion density equal to the remaining density after the inelastic parts have been removed. Using the depletion splitting method allows for smoother solutions of internal energy without excessive increases in the number of simulated collisions. Exchange probabilities for the reduced level number model are pre-calculated from a Larsen-Borgnakke model or some other model such as a state-to-state model and read from a data file during the initialization phase of the code. Results will be shown for simulations of diatomic gases. Comparisons will be made to Direct Simulation Monte Carlo and experimental results.

REFERENCES

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