MULTI-SCALE MODELS AND COMPUTATIONAL METHODS FOR AEROTHERMODYNAMICS

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The surface heat flux experienced by a spacecraft during its re-entry represents one of the main design parameters for rocket scientists. Its value must be accurately predicted in order to avoid mission failure and also to reduce the margins enabling to carry more payload. An accurate modeling of physical processes occurring in shock layers is deemed to be necessary. There, the flow experiences a sudden increase of temperature, pressure and density while crossing the shock wave. Atom and molecule collisions are enhanced leading to excitation of internal degrees of freedom and to molecular dissociation. For re-entry speeds typical of Lunar returns, ionization may also occur. Simulations of these flows are extremely complex because nonequilibrium phenomena occur in flow regions where the characteristic time-scales of collision processes become of the same order of magnitude as the ones of the flow. A correct modeling of aerothermodynamics flows is also crucial to interpret experimental data acquired in high enthalpy facilities, such as shock tunnels and plasma torches.

The computation of aerothermodynamic flows is usually performed by assuming that the atom and molecule internal degrees of freedom can be described in terms of Boltzmann distributions at their own temperatures (multi-temperature models - MT). Unfortunately this approach can be applied only in case of low departure from equilibrium. State-to-state (STS) collisional models have been proposed as alternative. Each internal energy level is considered as a separate pseudo-species, allowing for occurrence of non-Boltzmann distributions. The application range of STS models is therefore broader than that of MT models (no hypothesis on internal energy level distributions) allowing for a more accurate physical description. The computation of rate coefficients for each collisional process considered requires complex quantum mechanical calculations.

The application of STS models to 2D/3D flow calculations becomes computationally expensive because of the high number of equations to be solved (for each energy level, treated as a pseudo-species, a mass conservation equation has to be considered). One of the objectives of this thesis is to formulate reduced macroscopic physical models (suitable for the application to CFD problems) from STS models. Benchmarks, such as quasi 1D nozzle and normal shock flows, are considered since these simple testcases retain the main characteristics of actual aerothermodynamic flows. Up to now, research efforts have been focused on the rovibrational collisional model for the $N + N_2$ database of the Computational Quantum Chemistry Group of NASA Ames Research Center. Different coarse grain models (such as *bin* and *vibrational* collisional) have been formulated by lumping the original set of rovibrational energy levels (9390) into energy *bins*. Results for an expanding flow (see Fig. 1) show that an accurate description can be already obtained by using only 20-30 *bins*. At the same time, a comparison between computed and measured vibrational energy level population distributions (NASA EAST facility, see Fig. 2) has allowed for a partial validation of the reduced physical models developed.

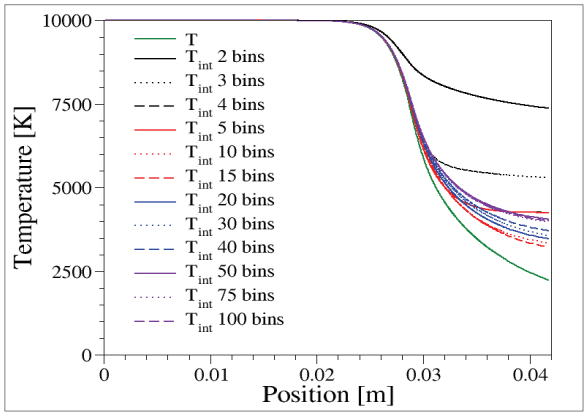

Figure 1 : Internal temperature along the axis of the nozzle of the VKI Minitorch facility

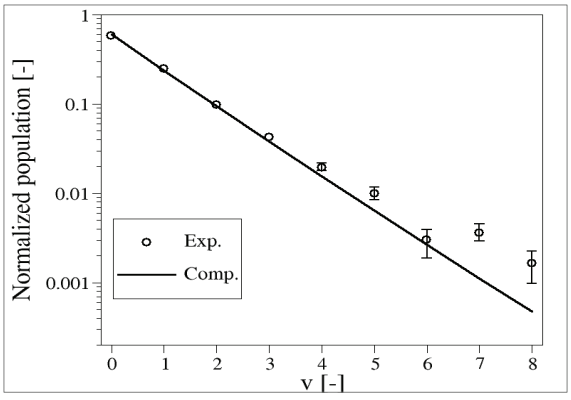

Figure 2 : Computed and meassured vibrational energy level populations.4 cm from at 2 the throat of nozzle of the NASA EAST facility