DIRECT SIMULATION MONTE CARLO FOR AEROSPACE APPLICATIONS

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In this work, we investigate high temperature gas-phase phenomena such as internal energy excitation and molecular dissociation under rarefied conditions characteristic of reentry flows. In the upper atmosphere, the local Knudsen numbers reach values high enough for significant translational non-equilibrium to prevail in the bow shock, the boundary layer and the wake flow of a reentry vehicle. Additionally, the strong compression in the bow shock causes vibrational energy modes of polyatomic molecules to become excited and for molecular dissociation to occur. These phenomena have a noticeable effect on the internal structure and stand-off distance of the bow shock, as well as on the surface heat flux.

The particle-based Direct Simulation Monte Carlo (DSMC) is used to model the aforementioned effects in a simplified flow configuration. The first part of this work consists of a review of the established models for internal energy exchange (Larsen-Borgnakke) and chemical reactions (Total Collision Energy) used in DSMC. For the purpose of this investigation, we are developing a dedicated DSMC code capable of simulating one-dimensional flows, including internal energy exchange and chemistry coupling. The test case to be simulated consists of a flow of molecular nitrogen being compressed through a normal shock wave. This causes the internal energy modes of N_2 molecules to be excited and leads to partial dissociation. Downstream of the shock, the relaxation towards post-shock equilibrium of the translational, rotational and vibrational temperatures, as well as the fraction of atomic nitrogen is monitored. A comparison is made between these DSMC simulations and equivalent CFD simulations obtained by means of a Navier-Stokes solver based on a multi-temperature model (Fig. 1). Special care will be taken to apply energy exchange terms and chemical reaction rate coefficients in the CFD simulations that are consistent at macroscopic scales with those used in DSMC.

In the future, the aim is to improve the existing models in DSMC for rotational and vibrational modes by using a reduced model developed from a detailed chemical mechanism based on rovibrational cross sections for reactions in nitrogen. These models will be based on the cross sections for the N3 system obtained from detailed quantum mechanical calculations obtained at NASA Ames Research Center. The N3 system consists of about 10000 rovibrational levels and its implementation in DSMC, even for simple types of flows, becomes a challenge, due to the large number of particles needed for populating all possible states in a realistic fashion. Consequently, our efforts will be directed towards developing a model for lumping together energy states lying close to one another and thus reducing the total number of levels required. A similar effort is already underway in developing such reduced models for continuum CFD solvers. The final goal will be again to compare simulations between consistent CFD and DSMC models.

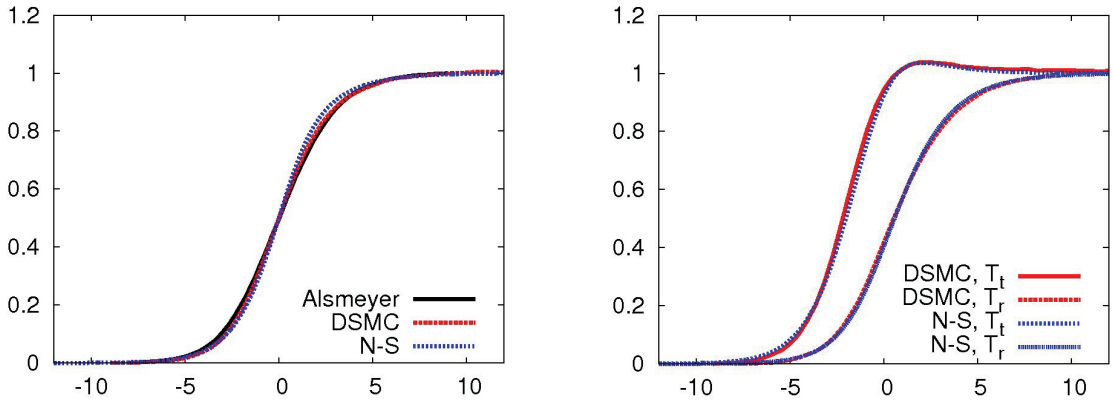

Figure 1 : Mach 1.71 shock wave: comparison between CFD and DSMC solutions, normalized profiles of density (left) and temperature (right)