

Modelling of of Titan-Like N₂-CH₄ Shocked Flows

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1 Introduction

Since the successful entry, descent and landing of the space probe Huygens on the surface of Titan in 2005, a renewed interest for additional missions to this satellite of Saturn exists. One of the more challenging phases of such a mission is the atmospheric entry phase, where large convective and radiative fluxes from the surrounding plasmas are withstanding by the spacecraft thermal protections. The modelling of relaxation processes behind such a shockwave allows a better understanding and predictability of such heat fluxes, and in particular from the ubiquitous CN Violet radiative system, which has a predominant contribution to the overall heat fluxes.

The atmosphere of Titan is composed from 98% N₂-2% CH₄, and therefore, chemical kinetics involving the N₂ molecule are predominant. Furthermore, as models of postshock relaxation processes, based on macroscopic/multitemperature models, are known to not have an accurate enough description of such physical processes, a hybrid macroscopic/state-to-state chemical model is proposed based on a recently proposed multiquantum state-to-state rate database for N₂ dissociation, developed by our research group.

2 Selection of adequate macroscopic and state-resolved chemical datasets

Using The Forced Harmonic Oscillator (FHO) theory [1], a database of multiquantum V-T and V-D rates for N₂-N₂ collisions has been produced, considering and upgraded manifold of vibrational energies, comprised of 61 quantum levels. This dataset is a considerable improvement over the more traditional first-order approaches like the SSH model, who fail at accurately predicting transition probabilities for high collision velocities such as the ones encountered behind a shock-wave, but also are incapable of predicting multiquantum rates. This state-to-state dataset has been validated against thermal dissociation rates from shock-tube experiments, showing an excellent simulation of such rates. For N₂-N collisions we consider the dataset from Esposito et al. [2], obtained using a QCT method, and who is also capable of accurately reproducing thermal dissociation rates for N₂ atom-diatom collisions.

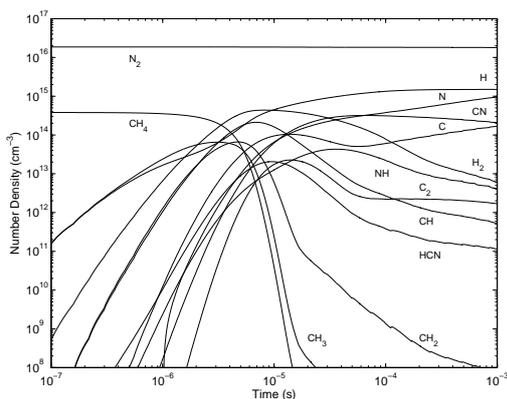
For the other processes, like the pathways for the dissociation of CH₄ and the creation of the various post-shock species, no complete state-to-state model exists, but a very detailed model has been recently proposed by Gökçen [3] for the specific topic of shockwaves modelling in Titan-like flows. Here we have selected as a first step the reduced 11 species (H, C, N, H₂, C₂, N₂, CH, NH, CH₂, CH₃, CH₄), 27 rates model, disregarding ionic species and reactions in this first approach.

Backward rates for this kinetic model have been calculated considering the detailed balance principle, considering $K_b = K_f/K_{eq}$. Reactions equilibrium constants have been obtained from equilibrium concentrations in a N₂-CH₄ plasma, which in turn have been calculated up to 50,000K using a Gibbs free energy minimization method. For the state-to-state dissociation rates of N₂, backward recombination rates have been likewise obtained using a detailed balance method [4].

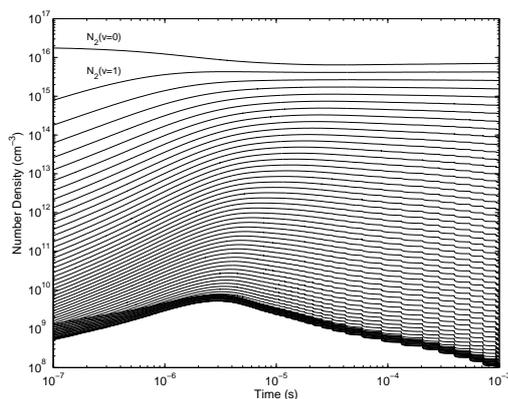
Energy balance has finally been considered in a traditional way, accounting for exchanges in the translational and internal modes with the enforcement of a total energy conservation. Temperature-dependent energies for macroscopic species have been calculated from NASA polynomial fits.

3 Simulation of relaxation processes downstream of a 5km/s shockwave

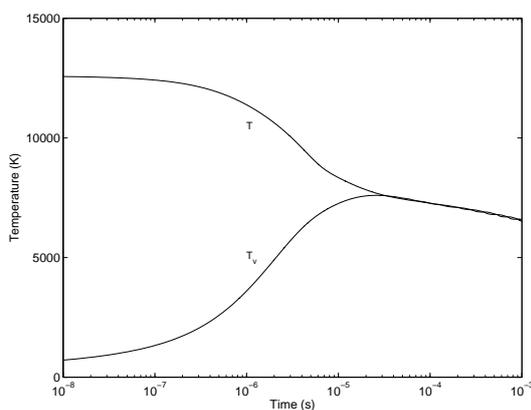
The numerical model has been applied to the simulation of the relaxation behind a shock-wave of 5km/s, at an initial pressure of 13Pa. The obtained results are presented in the figures below.



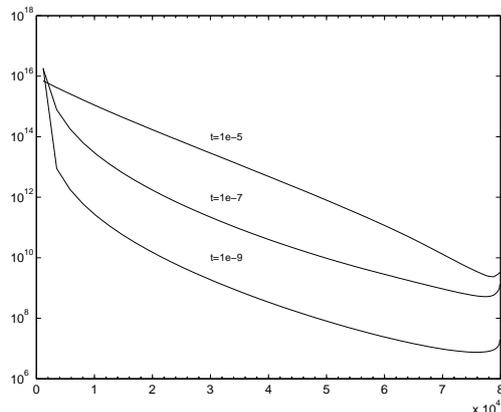
(a) Time-dependent macroscopic species concentrations. CH₄ is quickly cascaded into CH₃, CH₂, and CH, in the interval $t = (5 \times 10^{-5} - 5 \times 10^{-4})$ s.



(b) Time-dependent $N_2(v)$ levels concentrations. Equilibration to a Boltzmann vdf proceeds up to $t = 5 \times 10^{-5}$ s where higher levels start being depopulated by dissociation reactions.



(c) Time-dependent translational T and average internal energies (T_v). Equilibration is reached around $t = 5 \times 10^{-4}$ s.



(d) Time evolution of the Vibrational Distribution Function of N_2 , plotted as a function of vibrational level energy.

References

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- [3] Gökçen T. 2005 *J. Thermophys. Heat Transfer* 21 9.
- [4] Lino da Silva M. Guerra V. and Loureiro J. 2008 *Chem. Phys.* 358 123.