Topic 1

Reactivity, relaxation and dissociation of molecules in plasma modeling

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Detailed information on the dynamics and kinetics of molecular collisions are of key importance in accurate modeling of aerothermodynamics, combustion, laser and plasma physics. A discussion of the relevant problems, solutions and achievements will be presented, taking into account the need of complete data in the plasma modeling community.

1. Vibrational kinetics: the input data

In the plasma community it is nowadays well recognized the key role of vibrational energy exchanges among molecular species in plasmas [1]. Non-equilibrium conditions including vibrational energy are commonly studied in this field, and this implies the use of state-to-state (sts) data for all the relevant species of interest. In the past, simple models of vibrational energy transfer and dissociation from excited vibrational states have been used for this aim, and often continue to be used. However, it is now possible to calculate sts data accurately, with reasonable amounts of computational resources and with accurate interaction potentials [2,3,4]. These data can also include reaction, with production of new species with vibrational distributions quite different from the purely inelastic data. The insights and possibilities offered by these accurate and detailed data will be shown, with particular emphasis on the differences with simple models. Different methods are available, with specific features that have to be wisely studied, exploited and merged in order to get the most accurate and complete results [1,5], without neglecting the computational efficiency, which is a strict requirement, due to the large mass of calculations involved. A discussion about the use of these methods for both vibrational energy exchange with and without reaction and dissociation will be presented.

2. References

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