Vibrational Kinetics, electron dynamics and elementary processes in H_2 Plasmas for Negative Ion Production: Modelling Aspects

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One complex feature of the plasmas currently used and proposed for the production of hydrogen negative ions is the paramount role of the non equilibrium vibrational distribution function (vdf) of molecules and of the electron energy distribution function (eedf) of free plasma electrons. Under typical plasma conditions these two functions cannot be described by equilibrium laws. The complexity is enhanced by the impressive multiplicity of chemical processes whose parameters must be known in order to close the mathematical issue and deliver a full computer simulation. A typical solution method is based on an isotropic Boltzmann equation (BE) for the eedf mathematically coupled to the Master equation (ME) for the vdf. This technique has been used to deliver effective models for the multipolar negative ion sources for more than 20 years. As regards self-sustained discharges, a new layer of complexity is added by the electron production and loss kinetics. Of course, the BE/ME scheme can be modified to fit the more complex problem. A completely different approach is to use a Fluid model or a Particle in Cell/Monte Carlo simulation method for the charged particle transport. These solutions are very effective for modelling beyond the 0D case and allow a glimpse of the plasmadynamics without overlooking the fundamental coupling with the chemical aspects. Another important problem is the determination of the mostly unknown state-to-state electron/molecule and atom/molecule cross sections, e.g. by semiclassical methods and classical molecular dynamics calculations respectively. Further studies are still necessary to quantify the role of controversial reaction channels, such as the production of Rydberg molecular states by electron impact and the influence of these states on the negative ion yield. To illustrate the practical applications of some of these models different types of sources are investigated. The first one is a classical negative ion source in which the plasma is generated by thermoemitted electrons and a new computational scheme is presented to couple heavy particle and electron kinetics. Moreover models developed for RF inductive and parallel plate discharges are described.