Application of MCCC cross sections in collisional radiative models for molecular hydrogen: current status and outlook

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Population models are an important tool for interpreting observed plasma parameters or for predicting for known plasma parameters the plasma behavior. In plasmas used in fusion research the particle temperatures and densities can cover a wide range. Typically, the edge plasma of fusion devices is much cooler than the core plasma, resulting in the presence of atoms and molecules and thus a high complexity of the reaction kinetics. Together with the presence of strong density gradients, processes like Molecular Assisted Recombination or the transition from an ionizing to a recombining plasma regime can play a crucial role. Strong parameter gradients are also present in the negative hydrogen ion sources for neutral beam injection (NBI) at ITER. An ionizing plasma (T_e>10 eV) in the driver region is cooled down by a magnetic filter field to a recombining plasma with T_e≈1 eV close to the extraction system. Consequently, population models for atoms as well as for molecules are needed, being precise over a broad parameter range.

Collisional radiative (CR) models represent the most versatile type of a population model. A huge number of input parameters (reaction probabilities) are needed, in particular in the case of molecules where vibrational or rotational sublevels are present. Due to the presence of deuterium and tritium in fusion plasmas, the development of molecular CR models also for isotopomeres of H_2 is desirable, further increasing the data needs. The present results are based on the well-benchmarked Yacora CR models for atomic and molecular hydrogen, both being accessible also online via the tool Yacora on the Web.

In the last years large gaps in the available set of excitation cross sections for molecular hydrogen needed as input for CR models have been filled by a set of electron collision excitation cross sections, recently calculated by using the Molecular Convergent Close-Coupling (MCCC) method at Curtin University, Perth, Australia. In a common effort, the non-vibrationally resolved MCCC cross sections for the triplet system of H_2 were implemented in Yacora for H_2 and a benchmark was successfully performed versus results from a planar ICP discharge. An extension to the singlet system, including singlet-triplet mixing is planned next.

Further planned extensions made possible by the MCCC cross sections are the development of CR models for the isotopomeres of hydrogen, being of high relevance for fusion plasmas. Additionally planned is the development of ro-vibrationally resolved molecular CR models. Such models will be an important tool for determining – e.g. by means of emission spectroscopy – the rotational and vibrational temperature of the molecule which are important parameters for characterizing the plasma properties.