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Collisional radiative models for atomic and molecular hydrogen in the edge plasma of fusion devices

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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. The properties of the edge plasma in fusion devices as well as the processes taking place within this region are of great relevance for the overall behavior of a fusion plasma. Typically, the edge plasma 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 gradients in particle temperatures and densities, processes like Molecular Assisted Recombination or the transition from an ionizing to a recombining plasma regime can play a crucial role. 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.

Large gaps exist in the available set of molecular excitation cross sections needed as input for CR models. Even for the hydrogen molecule, the simplest existing neutral molecule, no complete data set of cross sections exists that includes vibrational sublevels, excited state-excited state reactions and the isotope effect. Recently a set of electron collision excitation cross sections, calculated by using the Molecular Convergent Close-Coupling (MCCC) method at Curtin University, Perth, Australia became available. 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.

An existing comprehensive set of dissociative and non-dissociative ionization cross sections for the ground state and electronically excited states of H_2, based on the semi-classical Gryzinski approach, is extended by data for D_2, T_2, HD, HT and DT. The total ionization cross sections for H_2 were successfully validated versus MCCC cross sections. The existence of cross sections for all isotopomeres opens the door towards the development of CR models for the isotopomeres of hydrogen.

The general availability of cross sections for the hydrogen atom is much better compared to the molecule. Open points are still present mainly regarding the connection of excited atomic states to the molecule or molecular ions. Nonteheless, the steady improvement and availability of data are important steps for increasing the reliability of model predictions for the edge plasma in fusion devices.

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