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Vibrationally and ro-vibrationally resolved collisional radiative modelling of molecular hydrogen: current status and outlook

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Collisional radiative (CR) models represent the most versatile type of population models used for determining 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. The situation is similar 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, CR models for atomic and molecular hydrogen are needed, being precise over a broad parameter range.

While the development of models for atomic hydrogen is mostly finished and well benchmarked models exist, the situation for molecular hydrogen is less definite. The reason is that due to the presence of vibrational and rotational sublevels a huge number of input parameters (reaction probabilities for collisional and radiative processes) are needed. Up to a few years ago mostly models resolving only the electronic states were applied due to the lack of appropriate reaction probabilities even for electron collision excitation. Even within the input used for these models large inconsistencies were present. Recently, some gaps in the available set of electronically and vibrationally resolved excitation cross sections for molecular hydrogen have been filled, shifting the main point of interest from electronically resolved models towards vibrationally or even ro-vibrationally resolved models. The presence of deuterium and tritium in fusion-relevant plasmas makes the development of molecular CR models desirable also for isotopomeres of H_2, further increasing the data needs.

Starting point for the present investigations are the well-known Yacora CR models for molecular hydrogen. A combined approach is followed, using three models with different levels of detail: an electronically resolved model for basic investigations on the kinetics of excitation and de- excitation of electronic molecular states, a vibrationally resolved model mainly for the reaction kinetics within the manifold of vibrational states within the electronic ground state X^1 and their impact on electronically excited states and a ro-vibrationally resolved Corona model for the Fulcher band transition ($d^3 \rightarrow a^3$). Final aim are well-benchmarked ro-vibrationally resolved models that can be applied to selected molecular optical emission bands over a broad range of plasma regimes. The current status of the models and the process of benchmarking them versus experimental data is introduced and current data needs are pointed out and discussed.

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