Atomic and Molecular data for collisional radiative modelling relevant to fusion

Dirk Wünderlich and Ursel Fantz
Max Planck Institute for Plasma Physics (IPP), Garching, Germany

Population models, predicting population densities of excited atomic or molecular states in dependence of the plasma parameters, are typically used for plasma diagnostics. One specific type of population models that can be applied over a wide range of plasma parameters are Collisional Radiative (CR) models. In CR models, exciting and de-exciting reactions for excited states in the atom or molecule are balanced. As a result, a huge number of input parameters (reaction probabilities) are needed; this number increases even more in the case of molecules where vibrational or rotational sublevels are present.

The plasma parameters of plasmas used in fusion research can cover a wide range. For example, the transition from the attached to the detached mode of the divertor plasma in tokamaks results in a strong reduction of the electron temperature (from ≈ 50 eV to below 1 eV) which implies the transition from an ionizing to a recombining plasma. 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 ≈1 eV close to the extraction system.

Consequently, the reaction probabilities included in CR models for these plasmas need to cover an energy range starting from close to the excitation threshold up to energies of more than 100 eV. Additionally, the transition from an ionizing to a recombining plasma can drastically shift the relevance of different excitation channels. Both, fusion machines itself and ion sources for NBI can be operated in different hydrogen isotopes. Different other particle species like He, Ar or N_2, Cs may be present in the plasmas, either as diagnostic gas or for modifying the properties of the plasma or the surfaces. It may additionally be necessary to include into the models processes including photons; for example in the case of a high ground state density self-absorption caused by optical thickness is significant.

CR models based on the flexible solver Yacora are available for several atomic and molecular species used in plasmas for fusion. The presentation discusses the available atomic and molecular data used as input in these CR models. While the general situation for light atoms is good, for molecules large gaps exist in the data basis of excitation cross sections. Even for the hydrogen molecule, the simplest existing molecule, no complete data set of cross sections exists that includes vibrational sublevels, excited state-excited state reactions and the isotope effect. The present available data set for the H_2 molecule is presented, including corrections and extensions performed in the last years. For the first time, cross sections calculated at Curtin University, Perth, Australia, using the Convergent Close- Coupling (CCC) method have been implemented into the Yacora CR model for H_2. The high relevance of the isotope effect will be highlighted. Additionally, a new service is introduced: Yacora on the Web is a web application, providing online access to the Yacora CR models for atomic and molecular hydrogen as well as for the helium atom.

Concluding, the presentation presents modelling activities with the focus on the low-temperature region of plasmas for fusion. Different CR models are available based on different sets of input data. The used input data is benchmarked at different plasma experiments.