§3. Critically Assessed Collisional Database for Hydrocarbons

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Hydrocarbon molecules are present in the cold periphery plasma regions of all fusion devices containing carbon based plasma facing materials. The generation of hydrocarbon molecules on carbon surfaces is the result of a complex surface chemistry and their release in the boundary plasma is induced by plasma-particle impact, thermal processes and other mechanisms. Chemical erosion is the most powerful mechanism for hydrocarbon release from carbon-based plasma facing materials for surface temperatures below 1000K[1].

Among the most intense hydrocarbon molecular influxes coming from the carbon surfaces into the plasma are those of CH_4, C_2H_2, C_2H_4, C_2H_6, C_3H_6 and C_3H_8, the mutual intensity ratios for which depends on the impact energy of plasma ions on the surface [2]. While the CH_4 is always the dominant fraction, the release of heavier hydrocarbons (C_2H_6 , C_3H_8) tends to increase with decreasing the ion impact energy (or plasma edge temperature). When entering the plasma edge (or divertor) region, characterized by low temperatures (e.g. below 10-15 eV in the divertor), the C_xH_y molecules become subject of a variety of collision processes with the plasma particles (e, H^+) and other edge plasma constituents (H, H_2). These collision processes determine the transport and radiative properties of hydrocarbon species in the plasma, as well as the transport of carbon atoms [3]. A successful modeling of the behaviour of hydrocarbon species in the fusion plasma boundary, as well as of their radiative properties, requires an accurate knowledge of the cross sections (or rate coefficients) for all their collision processes.

The cross section data information for the collision processes of hydrocarbon molecules and their ions, available prior to 1990, has been compiled by Ehrhardt and Langer [4](for the CH_y species only, y = 1-4) and Tawara et al [5]. No critical data assessment was attempted in these compilations. During the last decade, a large amount of new cross section data has been generated for the collision processed of C_xH_y molecules (x=1-3, $1 \leqq y \leqq 2x+2$) and their singly charged ions, which has allowed to generate a more complete cross section collection for these processes and perform a critical analysis of the data regarding their accuracy. We have, thus, undertaken to establish a critically assessed cross section database for the following processes of C_xH_y and $C_xH_y^+$:

1) electron impact dissociative excitation,
2) electron impact dissociative and non-dissociative ionization,
3) dissociative electron-ion recombination,
4) dissociative electron-ion excitation,
5) dissociative and non-dissociative electron capture by protons,
6) proton impact atom exchange reactions.

The processes listed above are the most important ones for the hydrocarbon species in the plasma edge (and divertor) regions if the neural particle density (H and H_2) is considered significantly smaller than the plasma density.

At the present stage, the database is completed for the processes 2), 3), 5) and 6) for all hydrocarbon species C_xH_y (x-1-3, $1 \leqq y \leqq 2x+2$) and $C_xH_y^+$, including determination of the cross sections for the most important dissociative channels. The determination of the branching ratio for many of dissociative ionization and recombination processes was a major effort, going beyond the available information in the literature. Several additional tools were used for resolving the branching ratio problem when only the total cross section for a given group of dissociative reactions was available.

The available data for the processes 1) and 4) are extremely scarce. Most of the data are limited to CH_4 and a few members of C_2H_y hydrocarbon series. There are, however, indications that the cross sections for these processes are considerable smaller than those for other electron impact processes in the energy region below 10eV. Fortunately, the present-day divertor studies focus mainly to the temperature region below 10-15 eV.

References:

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