

Collisional-radiative model for transport simulations of neutrals in detached conditions

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The importance of Eirene development for simulating the dynamics of neutrals and ions in the scrape off layer is discussed. As a first step the role of the reactions among molecular and atomic neutrals with ions in a edge tokamak plasma is investigated by using the solver for collisional radiative models Yacora [1]. Two different cases are considered with plasma parameters and reactions deduced from: i) EIRENE-EDGE2D simulations for JET cases [2], ii) the SOLPS-ITER simulations presented in Ref.[3] for a single-null EU-DEMO divertor scenario with kinetic neutrals. Atomic H , molecular H_2 and molecular ions H_2^+ hydrogen species are considered and the extension to deuterium species is envisaged via a proper scaling of reaction rates. The list of reactions includes molecular dissociation, induced ionization and molecular ion dissociation all by electron impact plus a charge-exchange reaction with bulk ions ($H_2 + H^+ \rightarrow H_2^+ + H$). A source term modeling gas puff provides molecules that dissociate into atoms and/or molecular ions, which are then ionized and/or dissociate again. At equilibrium H_2 density exhibits a peak at low temperature ($T < 3eV$) signaling weak molecule dissociation essentially due to charge exchange with protons. By increasing the temperature electron impact reactions become the main dissociation channel and suppress the molecular density. The model is then extended by including vibrationally resolved molecular states $H_2(v)$ and the corresponding electron-induced excitations and de-excitations among neighborhood states, which result to be the dominant reactions at low temperature. Hence, vibrational transitions and charge exchange reactions with bulk ions provide the main channels for the establishment of molecular and atomic equilibrium at low temperature. The relevance of charge exchange reactions with ions can be related with detachment control, while vibrational transitions are useful for setting up molecular spectroscopy as a proper diagnostic in the divertor region.

References

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