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The role of molecular reactions on power, particle and momentum balance during detachment

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It has been recognized, using divertor modelling cues, that molecular reactions can play an important role in divertor detachment through additional source/sinks of momentum, particles and energy. Such predictions, however, are difficult to confirm experimentally. We have developed such an experimental method and applied it to TCV discharges. The results support the importance of molecular processes and have implications on the handling of molecules in transport codes like SOLPS-ITER.

The increase of the Dα emission during detachment was quantified and used to infer the role of molecular reactions on power/particle balance during detachment. Based on previous work, higher-n Balmer lines were used to estimate the atomic contributions (recombination and excitation) to Dα. The difference to the total chordally-integrated Dα is used as an estimation of the molecular contributions. These are used to estimate the total hydrogenic radiation from plasma-molecule interactions, the intensity of Molecular Activated Recombination (MAR), and a measure of Molecular Activated Ionisation (MAI). The technique was applied to a TCV discharge, indicating that plasma-molecule interaction with D_2^+ (and/or D^-) can contribute up to 70% of the total Dα divertor emission in detached conditions during density ramps; while no increase beyond the atomic Dα is found during N_2 seeding. As no Dα enhancement is observed during N_2 seeded cases, the D^- and D_2^+ densities are concluded to be significantly lower. Possible reasons for this will be explored in this work.

D_2^+ (and/or D^-), alone, can account for significant radiative losses (up to 40% of all hydrogenic radiation) and significant ion sinks –MAR. The MAR onset occurs after detachment onset (power limitation) but before the onset of electron-ion recombination, (of smaller magnitude than MAR) throughout the discharge. Experimentally, we thus conclude that the influence of plasma-molecule interaction on particle and power balance can be significant. Additionally, SOLPS simulations indicate significant momentum removal can occur from plasma-molecule interaction. The implication of such molecular reactions for ITER/DEMO will be explored.

Analysis of Super-X MAST-U SOLPS simulations has indicated that plasma-molecule interactions, which are strongly enhanced by the large divertor chamber, have strong implications for opacity and its diagnosis. In addition, it is found that vibrational states are crucial in generating D^- and D_2^+ whose densities are strongly underestimated, in the standard use of SOLPS, in comparison to that obtained by post-processing SOLPS output through AMJUEL which matches the measured molecular contribution of Dα during the experiment. There is a need for continued comparisons of experiments with modelling to validate whether the physics involving molecules, as well as their influence on the plasma (particle/momentum/energy sources/sinks), are properly included in SOLPS.

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