The importance of plasma-chemistry in detached plasmas and the need for updated rates through CRM

Plasma-molecular interactions are pivotal in understanding the detachment process in fusion plasmas. These interactions involve collisions between molecules and atoms, contributing to both energy and momentum transfer from the plasma to the molecules. Furthermore, these collisions can lead to the rovibrational excitation of molecules, triggering subsequent interactions with the plasma, including the formation of molecular ions such as D2+ and D2- -> D- + D [1-3]. The behaviour of these molecular ions within the plasma is significant due to their multifaceted impact:

1. Excited hydrogen atom production, enhancing atomic hydrogen emission.
2. Molecular Activated Dissociation (MAD), leading to power losses and increased total dissociation rates.
3. Molecular Activated Recombination (MAR), resulting in the effective recombination of plasma ions and lowering the ion target flux.

Experimental observations on devices like MAST-U [4,5,6] and TCV [3], supported by novel atomic hydrogen emission spectroscopy analysis [7], underscore the critical role played by MAR in reducing the ion target flux, which is a defining factor of detachment. MAR begins at higher temperatures (<2.5 eV) compared to electron-ion recombination (EIR) (<1 eV). Moreover, MAR and MAD substantially contribute to atomic hydrogen emission, lead to significant power dissipation (up to 20% of the power entering the divertor), and emerge as the primary source of neutral atoms.

While SOLPS-ITER simulations agree with experiments up to the onset of detachment, disparities arise in the detached region of TCV and MAST-U when MAR and MAD become prominent [3,6]. These discrepancies stem from underestimations of the molecular charge exchange rate (D2 + D+ -> D2+ + D) in SOLPS-ITER. Adjustments and refinements of these rates have shown promise in enhancing agreement between experiments and simulations [8]. Applying these updated rates to reactor (STEP) simulations featuring a tightly baffled Advanced Divertor Concept (ADC) design [9,10,6], reveals their potential to significantly influence particle and power exhaust on a reactor. This influence could enable deeper levels of detachment than previously predicted.

The profound impact of plasma-molecular chemistry on detachment physics, particularly in divertors with alternative designs and strong baffling, necessitates improved rate calculations. This imperative step is crucial for enhancing predictions related to reactor exhaust, especially for devices like STEP and SPARC, which incorporate strongly baffled long-legged divertors.

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