Atomic and molecular processes in plasma surface interactions and boundary plasma science

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It was recognized as early as 1968 by Bo Lehnert [1] that a zone of powerful gas - plasma interaction, formed near highly PMI exposed surface elements, can be the key to solving the PSI issue for sustainable nuclear fusion reactor operation. Today the "divertor detachment" regime in tokamaks is characterised by strong volumetric exchanges of particles, momentum and energy, provided by a gas plasma interaction zone near target surfaces. For any given plasma state, and set of plasma material interaction processes (boundary conditions), this gas - plasma interaction can be fully quantified. Firstly, by resorting to highly accurate atomic/molecular (A&M) collision data. These are made available from many national atomic data centers and numerous data coordination and evaluation activities initiated and driven by the IAEA nuclear data section [2]. Secondly the high standards in (kinetic) transport applications from nuclear (neutronics, radiation) applications. Their full mathematical analogy to neutral particle transport in plasmas has been carried over into now quite mature fusion plasma boundary Monte Carlo codes.

Today the underlying details of the particular A&M data set in edge plasma models are often not made very transparent. In the present review we will try to publicly expose the most dominant A&M processes individually, their uncertainty levels today, and to quantify their physical effects on boundary plasma dynamics (notably on divertor detachment) as well as the potential loss of information in reduced (approximate), computationally simpler models derived from them. The focus is on collision processes involving fuel (H), ash (He), wall material (e.g., Be, W) and seeding particles (e.g., N_2), including molecules and molecular ions formed from them. It is shown that the dominant gas plasma friction in typical detached divertor conditions is to be expected from molecule - ion collisions, rather than from the often quoted resonant charge exchange. Direct contributions from molecules and their ions to atomic lines also complicate visible light spectroscopy as a divertor plasma diagnostic. Furthermore they may lead to quite unexpected kinetic isotope effects in the D-T mixture of a future reactor divertor plasma.

References:

[1] B. Lehnert *J. Nucl. Fus.* **8**, 173, (1968)
[3] IAEA Vienna, A&M Data Unit, https://www-amdis.iaea.org/index.php