Expansion of surface chemistry capabilities in EIRENE with a focus on ammonia production†

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Extrinsic impurity seeding is foreseen in future fusion devices such as ITER as the main means for divertor detachment control, in order to minimize the power fluxes to the divertor targets. Candidate gases for this purpose include Nitrogen (N), Neon (Ne), and Argon (Ar). Nitrogen, a strong radiator at divertor temperatures with a high ionization rate, is operationally preferred in small devices, as it tends to stay better confined in the divertor volume [1,2]. However, nitrogen injection into the plasma leads to ammonia formation. Although ITER is planning to use Ne injection, the alternative use of N is still being considered, hence it is important to assess the ammonia formation rate, as the presence of ammonia would require longer duty cycles to regenerate the cryopumps, and impacts tritium inventory management during the fusion operation phase.

To that effect, previous work [3] has been devoted to building a consistent reaction scheme for ammonia chemistry in plasma conditions such as those in the divertor and edge plasmas of tokamaks. Results from the first applications of that scheme have shown conclusively that ammonia and NHx radicals (here H stands generically for any hydrogen isotope) are destroyed in the plasma volume, and that the main formation mechanism occurs via surface chemistry. Moreover, dedicated experiments have shown that tungsten and stainless steel surfaces have a catalytic effect on ammonia formation in presence of an H2-N2 plasma [4]. They also indicate that, to a good approximation, the effects of surface processes leading to ammonia formation can be parametrized using a single number, \( f_{N\rightarrow\text{NH}_3} \), i.e. the fraction of incident N that will be reemitted as NH3, assuming a hydrogen-saturated surface state, and that NHx species all recycle as NH3. The \( f_{N\rightarrow\text{NH}_3} \) parameter depends on surface material, wall temperature, and the presence of other species in the plasma such as He or Ar.

In this paper, we build on the initial work from [3], using the Eirene Monte Carlo transport code, part of the SOLPS-ITER suite [5], to model the results from [4]. Eirene capabilities have been expanded to handle Arrhenius-style rates, non-elastic heavy-heavy collisions, and a variable recycling model. We search for the \( f_{N\rightarrow\text{NH}_3} \) parameter values which best match the measured ammonia formation rates. We then consider the effects of our surface ammonia chemistry model on existing nitrogen SOLPS-ITER tokamak simulations from AUG and JET.