

Nitrogen molecular break-up and transport simulations in the JET divertor

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Abstract The density of N^+ ions is predicted to decrease by 25 % and the density of N^{2+} ions to increase by 50 % if nitrogen is assumed to recycle from the divertor walls as molecules in partially detached JET L-mode plasma simulations performed with the 3D Monte Carlo trace impurity code ERO2.0 [1]. These findings are attributed to the kinetic energy gained by the molecular dissociation fragments in the Franck-Condon process and the resulting increase in plasma penetration of the atoms.

Introduction Nitrogen injection is used routinely for mitigating the heat loads to plasma-facing components in tokamaks with fully metallic walls [2]. Nitrogen seeding has been shown to increase energy confinement [3] and lead to smaller, more frequent edge-localized modes (ELMs) in high-confinement mode operation [4]. This study is focused on the effects of nitrogen molecular dissociation reactions on nitrogen transport.

Computational setup EDGE2D-EIRENE simulations of JET L-mode plasmas setup in earlier work by B. Lomanowski et al. [5] were used to produce background plasma files for ERO2.0. These simulations included deuterium as the main ion species, beryllium as an intrinsic impurity species and nitrogen as an injected impurity species. Nitrogen was injected as atoms from the low-field side target and assumed recycling off the divertor and main chamber walls. Nitrogen molecules were not included, as they cannot currently be simulated in EDGE2D-EIRENE. The low-field side mid-plane separatrix electron density was fixed to $2.0 \times 10^{19} \text{ m}^{-3}$ using feedback injection of D_2 into the private flux region. Drifts were not included due to numerical stability and convergence issues.

Two background plasmas were created: a trace impurity case [†] (5% total nitrogen radiation

[†][rmaenpaa/edge2d/jet/81472/sep0120#2](https://maenpaa.edge2d.jet/81472/sep0120#2)

fraction) and a radiative divertor case ^{††} (50% total nitrogen radiation fraction). The predicted low-field side target temperatures were 1.1 eV and 0.4 eV, respectively. These simulations were based on JET pulses 90419 (14.0 s to 16.0 s) and 90423 (15.5 s to 16.5 s). In both pulses, the toroidal magnetic field was 2.5 T, the plasma current 2.5 MA and the Ohmic power approximately 1.6 MW. Neutral beam heating power was applied at 1.8 MW, and the steady state was maintained for approximately 10 s.

ERO2.0 was used to investigate the impact of nitrogen molecular dissociation reactions on nitrogen transport. Three different ERO2.0 simulations were run for each background plasma. The first ERO2.0 simulation for a given background plasma included only nitrogen atoms. In the second simulation, nitrogen was injected as N₂ molecules, but nitrogen ions recycled as atoms. In the third simulation, nitrogen was injected as molecules and nitrogen ions also recycled as molecules. In ERO2.0, the dissociation of a nitrogen molecule imparts extra translational energy to the dissociation fragments (set here to a constant 2.0 eV, an approximate value based on experimental measurements [6]).

Results If the only source of molecular nitrogen is gas injection, then the impact of molecular dissociation reactions on the ion density distributions is negligible (within one standard deviation of the reference case with no molecules). This is due to the recycling source of nitrogen being approximately two orders of magnitude greater than the gas injection source in steady state. This result holds for both the trace impurity and radiative divertor case, and is consistent with previous studies [7].

If nitrogen is assumed to recycle as molecules, ERO2.0 predicts a 25% increase in the total N⁺ content of the plasma in the trace impurity case (Fig. 1). The total content of N²⁺ is predicted to decrease by 50%. The density of N⁺ and N²⁺ upstream of the LFS divertor entrance is also greater by approximately a factor of two than in the reference scenario, which indicates increased nitrogen divertor leakage. The line radiation from N⁺ and N²⁺ is predicted to increase by approximately 25% and 50%, respectively, if molecular recycling is assumed (Fig. 2). These findings are consistent with the increase in plasma penetration of the molecular dissociation fragments due to the gain in kinetic energy.

The total quantity of nitrogen ions in charge states 3+ to 7+ in the plasma increases by up to 50% (N⁵⁺) if all nitrogen is assumed to recycle as molecules. However, the analysis of higher nitrogen charge state densities is presently inconclusive due to numerical drifts in ERO2.0 that are introduced in the temperature gradient force calculation: the severity of these artefacts increases with the ion charge state. The numerical drifts cause an incursion of N³⁺

^{††} rmaenpaa/edge2d/jet/81472/sep0120#1

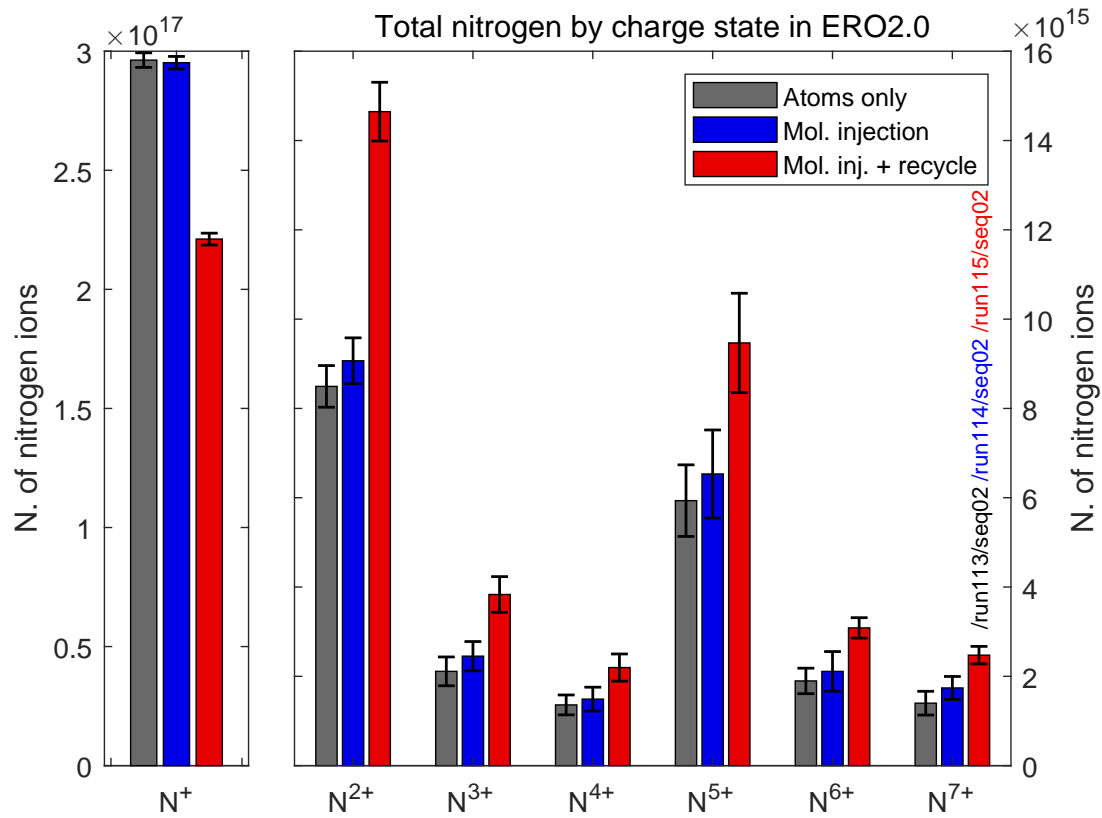


Figure 1: Total nitrogen ion content by charge state in the trace impurity case for the three different assumptions on nitrogen presence and recycling. Note the different vertical axis for N^+ .

and N^{4+} through the low-field side separatrix into the main plasma, peaking of the N^{5+} density around the X-point and accumulation of N^{6+} and N^{7+} to the high-field side of the main plasma. None of these three effects are seen in the EDGE2D-EIRENE simulations, or in the ERO2.0 simulations if the temperature gradient force is disabled.

Assuming molecular recycling produces qualitatively similar predictions in the radiative divertor case as in the trace impurity case. The N^+ content is reduced by approximately 25% and the N^{2+} content is increased by approximately 25%. Nitrogen divertor leakage also increased, as indicated by the approximately two-fold increase of N^{2+} density upstream of the low-field side divertor entrance. Increased line radiation from N^+ (by up to a factor of two) is observed in the radiative divertor case under the assumption of molecular recycling.

Comparisons to experiment are underway. To investigate whether higher nitrogen line radiation under the molecular recycling assumption leads to detachment with less nitrogen seeding, simulations with self-consistent fluid codes or with ERO2.0 coupled to fluid codes are needed. Ammonia formation reactions that may compete with nitrogen molecular recycling have not been included in these simulations and are an area of future work.

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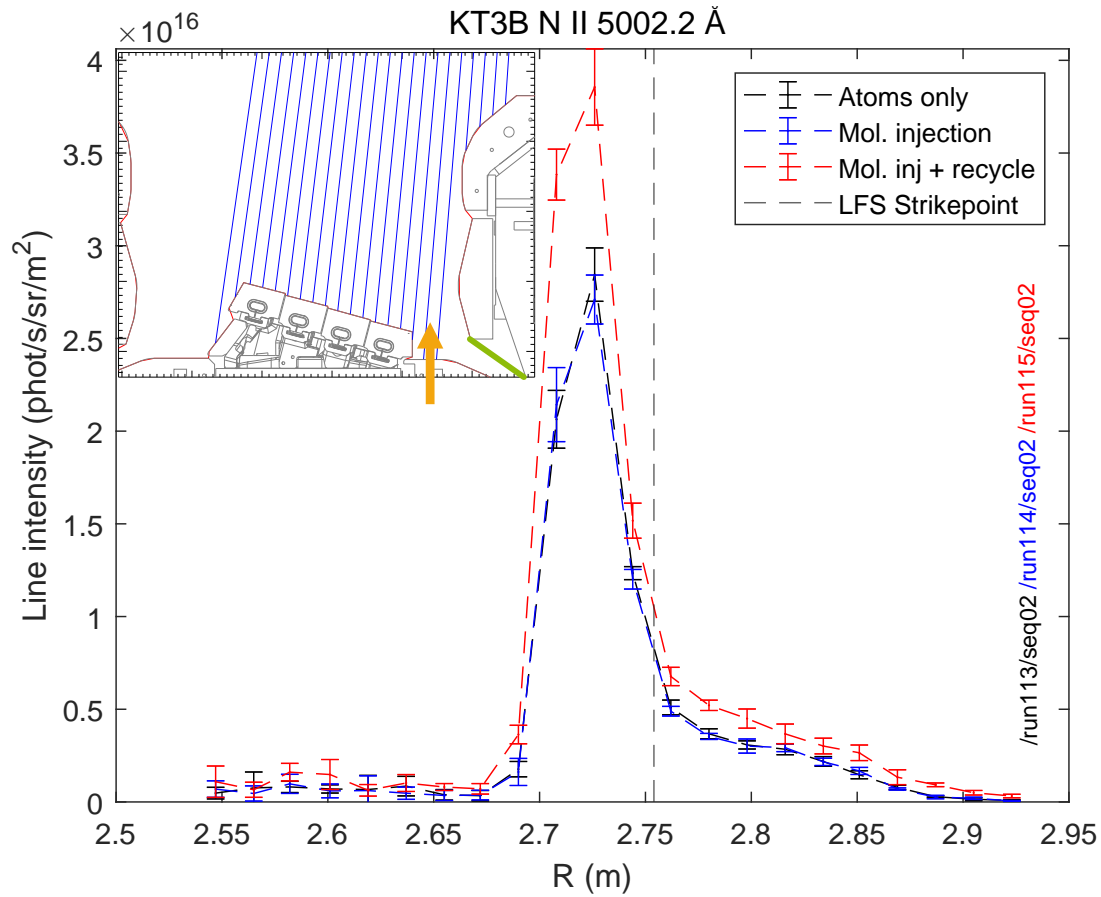


Figure 2: Synthetic diagnostic data for N^+ from the vertically viewing KT3B JET divertor spectrometer system. Error bars represent one standard deviation over several time steps, and lines are drawn to guide the eye. Insert shows the KT3B lines of sight in blue, the nitrogen injection location in orange and the pumping location in green.

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