# Characterization of Ar impurity screening across the H-mode pedestal in STEP using the JINTRAC code

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## Introduction

The Spherical Tokamak for Energy Production (STEP) programme aims to deliver a prototype fusion reactor that demonstrates net electricity production [1]. Impurity seeding will be essential to ensure a homogeneous distribution of heat fluxes in the form of radiation to the vessel walls and adequate divertor detachment. The amount of seeding must also remain compatible with good core performance and fusion yield, highlighting the importance of predicting impurity screening across the H-mode pedestal. In this study, we present integrated simulations of the new STEP SPP-002 baseline H-mode plasmas using the JINTRAC code. A scan of argon separatrix concentration has been performed at different separatrix electron densities to assess how much Ar impurity can be added to the core plasma before operational limits appear.

## Simulations set up

We focus on STEP SPP-002 DT H-mode flat top scenarios heated by 150 MW of electron cyclotron waves displaying high plasma core radiation fractions of 50% to 70%. This baseline corresponds to the engineering parameters: $\mathrm{R_{geo}} = 4.3\ \mathrm{m}, \mathrm{B_{geo}^{\phi}} = 2.98\ \mathrm{T}$ and $\mathrm{I_p} = 21\ \mathrm{MA}$. Turbulent dynamics are prescribed using the Bohm/Gyro–Bohm model feedback to a target fusion power value of $\mathrm{P_{fus}} = 1.68\ \mathrm{GW}$. Neoclassical transport has been studied using three different codes. NCLASS [2], which quickly solves the fluid equations force balance, but employs an approximated analytical formulation of the viscosity tensor. FACIT [3,4], a lightweight analytical model best suited for the Pfirsch-Schluter regime, and NEO [5], a computationally intensive code solving the linearized Drift-Kinetic equation. This comparison between reduced and computationally intensive transport models aims to assess the accuracy of lightweight approaches in predicting impurity transport for STEP H-mode plasmas. A parameter-space scan of electron and impurity separatrix densities is carried out to determine the optimal impurity seeding level consistent with pedestal physics, divertor detachment, and adequate core fusion performance. Scenarios are selected if they are stable and achieve the target fusion power.

**Effect of used neoclassical transport model**

To elucidate the impact of the chosen neoclassical transport model on the results, we first compare two runs of interest: an interpretive run with constant density and temperature profiles, where an Ar separatrix concentration of $c_{Ar,sep} = 1\%$ has been added, and a fully predictive simulation with $c_{Ar,sep} = 2.5\%$. The first of the two is shown in **Figure 1.**

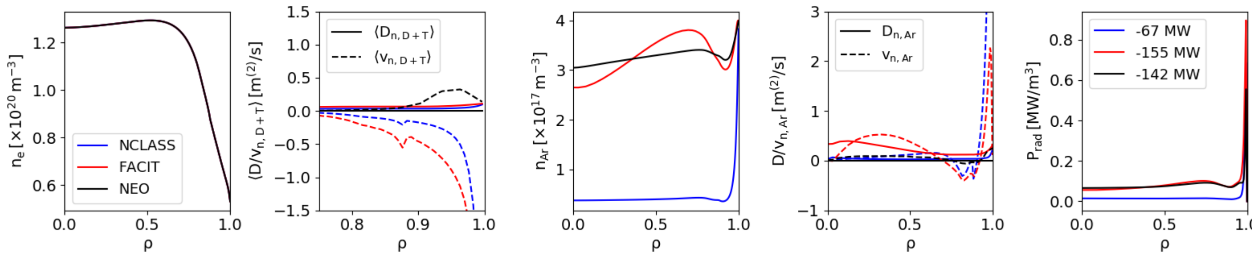


**Figure 1:** Interpretive DT run with $c_{Ar,sep} = 1\%$. From left to right: Electron density profile, averaged (D+T) main ion diffusivity and pinch velocity, Ar density profile, Ar neoclassical diffusivity and pinch velocity, and distribution of total radiation power.

This interpretive run shows clear differences in the Ar pinch velocity computed at the edge between NCLASS and FACIT/NEO. The large overestimation of the pinch by NCLASS leads to a large impurity screening that is not observed in FACIT and NEO, which agree quite well between each other in the impurity density distribution and radiation profile. Small differences can be observed between FACIT and NEO, but these don't seem to have a major impact on the predicted profiles. The fully predictive simulation can be seen in **Figure 2**.

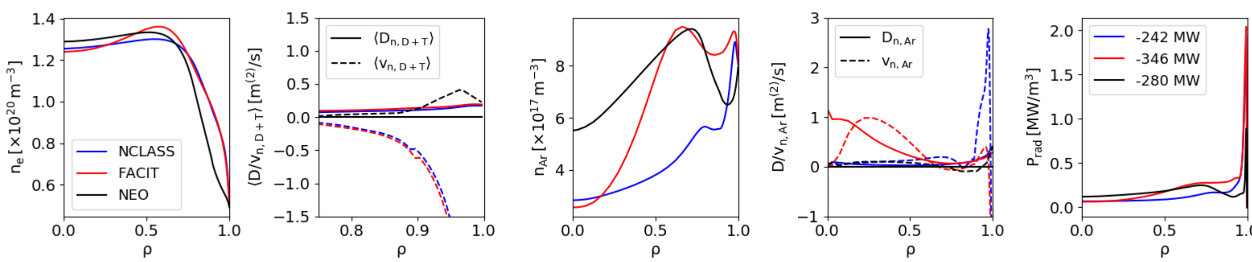


**Figure 2:** Predictive DT run with $c_{Ar,sep} = 2.5\%$. From left to right: Electron density profile, averaged (D+T) main ion diffusivity and pinch velocity, Ar density profile, Ar neoclassical diffusivity and pinch velocity, and distribution of total radiation power.

FACIT is currently only adapted to provide transport coefficients for impurities, and for this reason, NCLASS is additionally run for the main ions when FACIT is used. Therefore, the NCLASS and NCLASS+FACIT simulations agree quite well with each other in the prediction of the electron density profile, main ion diffusivity and pinch velocity. On the other hand, we observe a difference in the prediction of the electron density profile between NCLASS and FACIT with respect to NEO. NEO predicts a slight depletion of the electron density profile at the edge, and a softening of the gradients in that region. When we observe the main ion pinch, NEO correspondingly calculates an outward pinch velocity at the edge. Note that the transport computed by NEO is entirely represented by the pinch velocity, and as such, no neoclassical diffusivity is used in evolving the transport equations for NEO cases. This difference in electron and main ion density profiles, predicted by the different neoclassical transport models, has a direct impact on the transport of Argon in the core plasma. The large edge density gradients drive a large inward Ar pinch at the edge of the plasma for the NCLASS and FACIT cases, creating impurity accumulation in that region, whereas NEO displays an overall outward convection pinch for the impurity, leading to a smaller amount of Ar inside the separatrix. NCLASS also predicts a large outward pinch around $\rho \sim 0.97$, leading to strong Ar screening in the core, and a smaller total radiation of $\mathrm{P}_{\mathrm{rad}}^{\mathrm{NCLASS}} = 242$ MW. The three models also predict a local inward Ar pinch around $\rho \sim 0.8$, which creates a secondary accumulation zone visible in the Ar density profile. Finally, NEO and FACIT digress in the core Ar predictions, which we somewhat expect as we go away from the Pfirsch–Schlüter regime. Both FACIT and NEO display an outward Ar pinch creating a hollow impurity profile, however, FACIT does so with a notably larger magnitude, depleting the core from Ar, whereas NEO predicts a deeper impurity penetration. Since Ar radiates mostly in the edge region in the studied temperature range, NEO calculates an overall smaller radiated power of $\mathrm{P}_{\mathrm{rad}}^{\mathrm{NEO}} = 280$ MW compared to the value provided by FACIT of $\mathrm{P}_{\mathrm{rad}}^{\mathrm{FACIT}} = 346$ MW.

**Calculation of Ar separatrix concentration limit**

In this section we perform simulations with NCLASS and NEO to elucidate the Ar separatrix concentration limit compatible with core performance and divertor detachment. STEP specifications determine a limit for the cryopump tritium inventory of 400 g, which combined with a regeneration time of 30 mins yields a DT gas puff limit of $\Gamma_{\mathrm{DT}} = 9 \times 10^{22} \mathrm{part/s}$. Using two-point model estimations from [6], this gas puff limit corresponds to a separatrix electron density of the order of $\mathrm{n}_{\mathrm{e,sep}} \sim 5.5 - 6 \times 10^{19} \mathrm{m}^{-3}$. We have used this value as the upper limit boundary condition for the separatrix electron density in JETTO. In addition, we have considered a helium separatrix concentration of $\mathrm{c}_{\mathrm{He,sep}} = 10\%$ based on SOLPS estimates at the time. We have also focused on high ion density / low dilution cases. Two ion boundary conditions have been studied: $\mathrm{n}_{\mathrm{D}} = \mathrm{n}_{\mathrm{T}} = 1.6 \times 10^{19} \mathrm{m}^{-3}$ and $\mathrm{n}_{\mathrm{D}} = \mathrm{n}_{\mathrm{T}} = 2 \times 10^{19} \mathrm{m}^{-3}$. The pedestal structure is determined by the EPED1 model. The Ar concentration is then ramped in incremental steps until the simulation is no longer able to sustain the generated radiation power. The results can be seen in **Figure 3.**

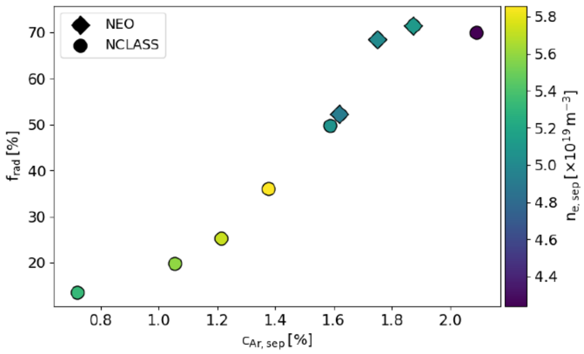


**Figure 3:** Radiation power fraction as a function of Ar concentration at the separatrix for the NCLASS and NEO neoclassical transport models.

For higher ion separatrix density, the achievable radiated fraction reached around $f_{rad} \sim 40$ % with an Ar separatrix concentration of $c_{Ar,sep} = 1.4$ %. At lower boundary ion density, higher radiation fractions of $f_{rad} \sim 70$ % can be obtained with Ar concentrations of $c_{Ar,sep} \sim 1.8 - 2$ %. Notably, NEO predicts a higher allowable $c_{Ar,sep}$ than NCLASS, which is in line with the predictive run displayed in Figure 2. The inward pinch at the separatrix predicted by NCLASS generates a radiation layer at the edge, which ultimately is the limiting factor determining the allowable edge impurity concentration.

## Conclusions

NEO, FACIT and NCLASS differ in the computed neoclassical transport coefficients in the pedestal region, which leads to different Ar screening factors and radiation profiles. NEO provides a softening of the main ion density gradient, which leads to a small outward pinch at the separatrix for Ar. On the other hand, FACIT and NCLASS predict stronger main ion density gradients at the edge, leading to an inward pinch for Ar impurity in that region. Since Ar radiates aggressively in the edge plasma layer, ultimately being the limiting factor to how much Ar can be added, in turn this reveals different limits for Ar concentration at the separatrix predicted by the three models. Notably, NEO predictions show that a $f_{rad} \sim 70$ % can be achieved at $c_{Ar,sep} \sim 1.8$ % and at a higher ion edge density of $n_D = n_T = 2 \times 10^{19} m^{-3}$. To obtain the same result with NCLASS on the other hand, we need to increase $c_{Ar,sep}$ to 2 % and reduce $n_D = n_T$ to $1.5 \times 10^{19} m^{-3}$.

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