Transport of collisional impurities with flux-surface density variation in stellarator plasmas

S. Buller\textsuperscript{1}, H.M. Smith\textsuperscript{2}, P. Helander\textsuperscript{2}, A. Mollén\textsuperscript{2}, S.L. Newton\textsuperscript{3} and I. Pusztai\textsuperscript{1}

\textsuperscript{1}Chalmers University of Technology, Dept. Physics, SE-41296 Gothenburg, Sweden
\textsuperscript{2}Max-Planck-Institut für Plasmaphysik, 17491 Greifswald, Germany
\textsuperscript{3}CCFE, Culham Science Centre, Abingdon, Oxon OX14 3DB, UK

Corresponding Author: bstefan@chalmers.se

Abstract:
Highly-charged impurities both dilute plasmas and lead to radiation losses, and thus cannot be allowed to accumulate in the center of a magnetic confinement fusion reactor. For stellarators, the picture has been particularly pessimistic, as early theoretical results predicted impurity accumulation for inward-pointing electric fields, which is the expected operational scenario for a stellarator-based reactor. However, these results were based on overly simplistic collision operators; recent neoclassical calculations with Fokker-Planck or mass-ratio expanded collision operators have shown that the transport of collisional impurities is in fact independent of the radial electric field\cite{1, 2} – unless the impurity density varies on the flux-surface\cite{3, 4}. Such variation can arise due to numerous effects, which highly-charged impurities are particularly sensitive to. In this work, we use the transport coefficients derived in Ref. \cite{3} to numerically optimize the impurity density on the flux-surface to yield minimal or maximal impurity accumulation in a case based on Wendelstein 7-X. This process provides bounds on the effects of the hard-to-measure impurity variation, and can potentially provide hints to how this impurity variation should be modified with suitable experimental actuators to avoid impurity accumulation.

1 Introduction

Highly-charged impurities cannot be allowed to accumulate in the center of a fusion plasma. In stellarators, these highly-charged impurities have been predicted to transport strongly in the direction of the radial electric field, which is typically expected to be inward in future stellarator reactors.

However, these expectations were based on calculations which model the collisions between particles with a simple pitch-angle scattering collision-operator\cite{5}. This is an inadequate model for treating highly-collisional impurities\cite{6}, which is the relevant collisionality regime for highly-charged impurities. For typical Wendelstein 7-X (W7-X) plasmas, this occurs when $Z \gtrsim 20$, where $Z$ is the charge number of the impurity. When the full Fokker-Planck collision operator is used, the transport of impurities becomes independent of the radial electric field at high-collisionality\cite{1}, and accumulation can be avoided.
For analytical calculations, the full Fokker-Planck operator is often approximated with a simpler operator. For heavy impurities, it can be expanded in the mass-ratio between the impurities and the bulk ions, which also yields impurity transport independent of the radial electric field – both when the bulk ions are collisional \[7\] and in a low collisionality \(\sqrt{\nu}\) or \(1/\nu\) regime\[1, 2\]. These mixed-collisionality regimes, with low-collisionality bulk and high-collisionality impurities, are the relevant regimes for tungsten impurities in a future stellarator reactor.

Highly-charged impurities are also more susceptible to developing density variations on the flux-surface. Such variations can arise due to the sensitivity of these highly-charged impurities to even slight electrostatic-potential variation, which can arise in stellarators due to trapping-effects\[8\] or fast particles\[9,10\].

In Refs. \[3, 4\], the analytic theory of Refs. \[1, 2\] was extended to include such effects. In particular, eq. (4.6)–(4.9) and (5.6) in Ref. \[4\] gives the transport coefficients of the impurity flux as functionals of the impurity density variation on the flux-surface. These expressions allow us to numerically optimize the impurity variation on the flux-surface to meet various criteria, such as minimizing the impurity peaking factor.

In this contribution, we present impurity variations that minimize and maximize the impurity peaking factor for a W7-X case. This work thus provides upper and lower bounds to the impurity peaking factor due to neoclassical transport. We find that both impurity accumulation and expulsion are possible in both cases, depending on the impurity density variations.

### 2 Theoretical formulation

From Eq. (4.5) in Ref. \[4\], the impurity flux can be written as

\[
\frac{\langle \vec{f}_z \cdot \nabla \psi \rangle}{\langle n_z \rangle} = D_\Phi \frac{e}{T} \frac{\partial \langle \Phi \rangle}{\partial \psi} - \frac{D_{N_z}}{Z} \frac{\partial \ln N_z}{\partial \psi} - \frac{D_{n_i}}{\partial \psi} - \frac{D_{T_i}}{\partial \psi},
\]

where \(D_\Phi, D_{N_z}, D_{n_i}\) and \(D_{T_i}\) are known quantities, with \(D_\Phi = -D_{N_z} - D_{n_i}\); see (4.6)–(4.9) and (5.6) in Ref. \[4\].

Here, \(\langle \cdot \rangle\) is the flux-surface average; \(n_z\) is the impurity density, which is allowed to vary on the flux-surface; \(n_i\) the bulk ion density; \(T_i = T_z\) is the bulk ion and impurity temperature; \(\psi\) is a flux-surface label; \(\Phi\) the electrostatic potential; \(N_z = n_z e^{Z e \Phi / T}\), with \(\tilde{\Phi} = \Phi - \langle \Phi \rangle\); \(Z\) is the charge number of the impurity. The flux-surface function \(N_z\) is known as the pseudo-density. It is related to \(\langle n_z \rangle\) by

\[
\langle n_z \rangle = N_z \langle e^{-Ze\Phi / T} \rangle,
\]

and will be used as a proxy for the actual density – which is valid provided that \(\langle e^{-Ze\tilde{\Phi} / T} \rangle\) does not vary too strongly with radius.

\(^1\)The impurities can also self-consistently set up such variation to satisfy parallel momentum balance in the presence of a strong friction-force\[10\], although this scenario will not be considered here.
We define the peaking-factor of the impurity pseudo-density as the gradient of \( \frac{d \ln N_z}{Z d \psi} \) that gives \( \langle \vec{\Gamma}_z \cdot \nabla \psi \rangle = 0 \), which determines the steady-state \( N_z \) profile in the absence of particle sources. The peaking factor can thus be calculated in terms of the transport coefficients \( D_X \) as

\[
- \left. \frac{d \ln N_z}{Z d \psi} \right|_0 = - \frac{D_{\Phi}}{D_{N_z}} \frac{e d \langle \Phi \rangle}{d \psi} + \frac{D_{n_i}}{D_{N_z}} \frac{d \ln n_i}{d \psi} + \frac{D_{T_i}}{D_{N_z}} \frac{d \ln T_i}{d \psi} = \frac{e d \langle \Phi \rangle}{T d \psi} + \frac{D_{n_i}}{D_{N_z}} \left( \frac{d \ln n_i}{d \psi} + \frac{e d \langle \Phi \rangle}{T d \psi} \right) + \frac{D_{T_i}}{D_{N_z}} \frac{d \ln T_i}{d \psi} \tag{3}
\]

With this definition, a negative peaking factor corresponds to a hollow \( N_z \) profile.

To avoid impurity accumulation, we seek to find an impurity density \( n_z \) that minimizes (3). We restrict the problem to a finite number of degrees of freedom by expressing \( n_z \) in terms of a truncated Fourier-expansion

\[
n_z(\theta, \zeta) = a_{00} f_{00}(\theta, \zeta) + \sum_{n=1}^{N} \left[ a_{n0} f_{n0}(\theta, \zeta) + b_{n0} g_{n0}(\theta, \zeta) \right] + \sum_{n=-N}^{N} \sum_{m=1}^{M} \left[ a_{nm} f_{nm}(\theta, \zeta) + b_{nm} g_{nm}(\theta, \zeta) \right], \tag{4}
\]

where the basis functions

\[
f_{nm}(\theta, \zeta) = 1 + \epsilon + \cos (m \theta - N_p n \zeta),
\]

\[
g_{nm}(\theta, \zeta) = 1 + \epsilon + \sin (m \theta - N_p n \zeta) \tag{5, 6}
\]

are chosen to be strictly positive (\( \epsilon > 0 \)) as the transport coefficients as derived in Ref. [4] diverge for \( n_z = 0 \). Here, \( \theta (\zeta) \) is the poloidal (toroidal) Boozer angle, with \( N_p \) the number of toroidal periods of the stellarator. To avoid unrealistically sharp variation in \( n_z \) and to limit the dimensionality of the problem, we restrict ourselves to \( N = M = 3 \), which corresponds to 49 Fourier coefficients to optimize. We eliminate one of the degrees of freedom (the \( n = m = 0 \) mode) by setting the impurity content on the flux-surface through \( \langle n_z \rangle \). We furthermore impose a non-linear constraint \( n_z > 0 \), which is needed since the coefficients \( a_{nm}, b_{nm} \) can be negative. The optimization is done by repeatedly generating random initial Fourier coefficients, and applying the gradient based method-of-moving-asymptotes [11], as implemented in the python version of the nonlinear-optimization package NLOpt [12]. This yields the local minima around the random initial conditions, and the best of these minima is taken as a best guess for the global minimum.

3 Results

We consider a case based on a W7-X standard configuration vacuum field, at normalized radius \( r_N = 0.6 \). Here, \( r_N = \sqrt{\psi_l/\psi_{LCS}} \), where \( \psi_l \) is the toroidal flux and \( \psi_{LCS} \) the toroidal flux at the last-closed flux-surface. We use \( \frac{e d \Phi}{T d r_N} = 1.03, \frac{d \ln n_i}{d r_N} = -0.297 \) and \( \frac{d \ln T_i}{d r_N} = -0.824 \). The magnetic geometry, bulk ion temperature and density, and radial electric field is taken from Ref. [13], although we deviate from the scenario in Ref. [13].
by considering a non-trace impurity with \( Z = 24 \) and \( \langle n_z \rangle / n_i = 10^{-3} \). The radial electric field is therefore not entirely self-consistent. However, our \( n_z \) optimization will turn out to be rather insensitive to the exact value of \( d\langle \Phi \rangle / d\psi \), as will be shown below.

![Figure 1: The initial \( n_z \) (left) and the \( n_z \) that minimizes impurity accumulation (right), for the W7-X equilibrium. Top row: the best \( n_z \) found. Bottom row: \( n_z \) found by starting from an initially homogeneous \( n_z \). The peaking factor and the \( D_X/D_N \) are given in the subfigure headings. The contours are of the magnetic field strength, with values in tesla.](image)

We ran the local optimization from 100 random initial \( n_z \). The best \( n_z \) thus obtained is presented in the top row of Figure 1, together with the corresponding initial \( n_z \) and peaking factors. For reference, the optimal \( n_z \) obtained by starting from an initially homogeneous \( n_z \) is shown in the bottom row of Figure 1.

As seen in Figure 1, the best \( n_z \) has a relatively simple form, with impurities strongly localized around the halfway point of the toroidal section. This feature arises when running the optimization from most of the random initial \( n_z \), and is generally correlated.
with a lower peaking factor – although merely having this feature is not a sufficient condition for minimizing the peaking factor, as will be shown in Section 3.1. In the result of the optimization from a homogeneous initial \( n_z \), this feature does not appear, and the peaking factor takes a somewhat smaller negative value. On the other hand, the flux surface variation of the impurity density is more modest in this case, and may be possible to produce in an experiment, since it is better correlated with the magnetic field on the flux surface.

To better understand what sets the \( n_z \) with the lowest peaking factor, we investigated the individual transport coefficient ratios: \( D_{n_i}/D_{N_z} \) and \( D_{T_i}/D_{N_z} \). As seen above the subfigures in Figure 1, the optimization mostly decreases \( D_{n_i}/D_{N_z} \) – which has the effect of increasing \( D_{\Phi}/D_{N_z} = 1 - D_{n_i}/D_{N_z} \) by the same amount – while it also increases \( D_{T_i}/D_{N_z} \) by roughly half of \( D_{n_i}/D_{N_z} \). In fact, we find that, \( D_{T_i} \approx -0.5D_{n_i} \) to within 2\% in most cases. This is consistent with the case of a homogeneous \( n_z \) – where the relation \( D_{T_i} = -0.5D_{n_i} \) is exact – and also with the findings of Ref. [4], where it was determined that \( D_{T_i} \approx -0.5D_{n_i} \) for various scenarios with non-homogeneous \( n_z \).

If we insert the assumption that \( D_{T_i} \approx -0.5D_{n_i} \) into the expression for the peaking factor, (3) we find

\[
\begin{align*}
-\frac{d \ln N_z}{Z d\psi} |_{0} & \approx \frac{e}{T} \frac{d \langle \Phi \rangle}{d\psi} + \frac{D_{n_i}}{D_{N_z}} \left( \frac{d \ln n_i}{d\psi} + \frac{e}{T} \frac{d \langle \Phi \rangle}{d\psi} - \frac{1}{2} \frac{d \ln T_i}{d\psi} \right),
\end{align*}
\]

which implies that when the quantity inside the round brackets is positive (negative), the optimum \( n_z \) should minimize (maximize) \( D_{n_i}/D_{N_z} \). This quantity is positive in the case considered here, which implies that the optimization procedure for the peaking factor should be equivalent to minimizing \( D_{n_i}/D_{N_z} \), and thus equivalent to maximizing \( D_{\Phi}/D_{N_z} = 1 - D_{n_i}/D_{N_z} \) or \( D_{T_i}/D_{N_z} \approx -0.5D_{n_i}/D_{N_z} \). This suggests that the \( n_z \) optimization will not depend on the exact value of \( d\langle \Phi \rangle/d\psi \), as long as the quantity inside the brackets is far from zero – although the actual value of the peaking factor is of course sensitive to \( d\langle \Phi \rangle/d\psi \).

It is thus of interest to find the \( n_z \) that maximizes or minimizes \( D_{n_i}/D_{N_z} \). Such \( n_z \) are displayed in Figure 2, where we also display the \( n_z \) that maximize or minimize \( D_{T_i}/D_{N_z} \) in order to validate the \( D_{T_i}/D_{N_z} \approx -0.5D_{n_i}/D_{N_z} \) assumption. From the first column in Figure 2 we see that the \( n_z \) that minimizes \( D_{n_i}/D_{N_z} \) is similar to the \( n_z \) that minimizes the peaking factor, as expected. Although the \( D_{n_i}/D_{N_z} \) minimization only leads to \( \sim 10\% \) reduction in \( D_{n_i}/D_{N_z} \), this is enough to change the role of \( d\langle \Phi \rangle/d\psi \), so that an inward electric field reduces the peaking factor. This effect may be even more pronounced in other machines, as an optimization with an LHD-like equilibrium showed a reduction in \( D_{n_i}/D_{N_z} \) by \( \sim 85\% \).

The third column in Figure 2 shows the \( n_z \) that maximizes \( D_{n_i}/D_{N_z} \). This maximization has more drastic effects on the transport coefficients, and the \( n_z \) features complex structures with more localized peaks. The \( D_{n_i}/D_{N_z} \) maximization also breaks the \( D_{T_i}/D_{N_z} \approx -0.5D_{n_i}/D_{N_z} \) assumption. This effect is especially strong when the optimization starts from a homogeneous \( n_z \).

The second and fourth columns of Figure 2 show the corresponding \( D_{T_i}/D_{N_z} \) maximization and minimization. The resulting peaking-factors and \( n_z \) are similar to the
FIG. 2: The $n_z$ that minimizes or maximizes $D_{n_i}/D_{N_z}$ or $D_{T_i}/D_{N_z}$. From left to right: minimize $D_{n_i}/D_{N_z}$, minimize $-D_{T_i}/D_{N_z}$, maximize $D_{n_i}/D_{N_z}$, maximize $-D_{T_i}/D_{N_z}$. Top row: the best $n_z$ found in the optimization. Bottom row: homogeneous initial $n_z$.

The corresponding $D_{n_i}/D_{N_z}$ optimization, although the exact details deviate. Part of this deviation is likely due to the fact that our procedure does not establish the global optimum, and only a best local optimum out of a number of random trails: thus, the $D_{n_i}/D_{N_z}$ and $D_{T_i}/D_{N_z}$ optimization will find different $n_z$ depending on the local optima sampled. However, even when the $D_{n_i}/D_{N_z}$ and $D_{T_i}/D_{N_z}$ start from the same initial, homogeneous $n_z$, the results deviate, so the difference between the $D_{n_i}/D_{N_z}$ and $D_{T_i}/D_{N_z}$ responses also plays a role.

3.1 Sensitivity to different modes

As the best $n_z$ has a relatively simple form, we are lead to investigate how many of the 48 unconstrained modes actually play a significant role in the optimization. In Figure 3 we show the effect of a truncation, where modes with amplitude below a given threshold are removed. From the bottom figure, we see that the $n_z$ modes span a large range of amplitudes, and that one mode in the “best” (randomly initialized) case is much larger than the rest. However, while this large-amplitude mode dominates the structure and amplitude of $n_z$ modes with 50 times smaller amplitudes are crucial for the optimization, as can be seen from the large increase in $D_{n_i}/D_{N_z}$ (above even the homogeneous-$n_z$ value of $-1$) when coefficients smaller than $2 \times 10^{-2}$ are truncated. This occurs at around 10 retained modes. This is in contrast with the optimal $n_z$ initiated from a homogeneous distribution, where only the largest and second largest mode seem to have a notable effect on the optimization.

In Figure 4 we show the coefficients of the different modes in the $n_z$ that minimize
FIG. 3: Top: The effects on $D_{ni}/DNz$ of truncating modes with amplitude below a threshold. Bottom: the number of untruncated modes at a given threshold. “Homogeneous” and “best” refers to $n_z$ resulting from the homogeneous initial conditions, and the best found $n_z$, respectively.

$D_{ni}/DNz$. For the best $n_z$, we see a clear dominance of $m = 0$ modes, which is consistent with the simple shape of the optimal $n_z$. Note the SymLog scale on the color-scale. As this $n_z$ optimum depends on precise values of such a large number of modes, it is unlikely that it is practically feasible to realize an exact enough match in experiments. Thus, this optimization is perhaps only useful for estimating bounds of neoclassical transport. In contrast, the $n_z$ optimized from an initial homogeneous $n_z$ appears sensitive to only a few variables, and may thus be a more suitable optimization target for an experiment. Future work is needed to find a function space such that elements in the space correspond to $n_z$ that are experimentally realizable, so that the optima in this space corresponds to situations that can occur in experiments.

4 Conclusions

Recently developed analytic expressions for the neoclassical transport coefficients of a heavy impurity in a stellarator plasma allow for the effects of flux surface variation of the impurity density. We have numerically explored the ability to reduce impurity accumulation by optimizing this impurity density variation, in a W7-X based equilibrium.

We extremized the ratios of transport coefficients $D_{ni}/DNz$ and $DTi/DNz$, where maximizing either of them roughly corresponds to minimizing the other, since we find that $DTi \approx -0.5D_{ni}$. When this approximation holds, minimizing (maximizing) $D_{ni}/DNz$ corresponds to finding the $n_z$ that yields the least (most) impurity accumulation. These
optimizations can thus provide upper and lower bounds to the impurity accumulation due to neoclassical transport. In the cases considered, when the flux-surface variation is represented by 49 Fourier modes, the resulting impurity peaking factors in W7-X thus span a range of roughly $[-0.24, 1.1]$ – although these bounds come from $n_z$ that may not be realized in experiments, and that are sensitive to a large number of modes.

Progressing from the simple proof-of-concept optimization presented here to more comprehensive studies accounting for available experimental actuators for flux surface variation of impurities, or spanning a larger parameter space, presents no fundamental difficulties, as the optimizations are reasonably inexpensive, and further non-linear constraints can be specified in the optimization framework.

Acknowledgements This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

References