On impurity transport calculations in stellarators

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Outline

- Introduction to impurity transport in stellarators
- Neoclassical calculations with equilibrium electrostatic potential variations $\Phi_1$
- $\Phi_1$ in linear gyrokinetic modelling
- Summary
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Impurity accumulation is a concern for stellarators,
e.g. \( \Rightarrow \) radiation collapse.

Radiative collapse: [Fuchert et al., internal meeting IPP Nov 2017]
If (locally) \( P_{\text{rad}} > P_{\text{heat}} \): \( dW/dt < 0 \)
- Either new (local) equilibrium or collapse.
- Complex process if impurity radiation is involved.

Limits the operational space of stellarators (critical density).

[Burhenn et al., Nucl. Fusion (2009)]
[Giannone et al., PPCF (2000)]

\[ n_{\text{crit}} \left[ 10^{19} / \text{m}^3 \right] \begin{align*}
Z_{\text{eff}} \sim 1.5, & f \sim 2 \% \\
Z_{\text{eff}} = 3, & f \sim 7 \% \text{ (carbon)}
\end{align*} \]
Neoclassical impurity accumulation

**In a tokamak (toroidal symmetry)**

- The Lagrangian is independent of the toroidal angle. Additional constant of motion.
- The neoclassical particle fluxes are intrinsically ambipolar \( \Rightarrow \) cross-field transport not affected by \( E_r = -d\Phi/dr \) (except centrifugal and Coriolis forces if strong rotation).

**In a stellarator (broken toroidal symmetry)**

- Helically trapped particles can drift out of the plasma \( \Rightarrow \) collisionless trajectories can leave the confined region.
- \( 1/\nu - , \sqrt{\nu} - \) regimes with enhanced neoclassical transport.
- Radial electric field \( E_r \) restores ambipolarity.
- \( E_r \) often points radially inwards \( \Rightarrow \) **Impurity accumulation.**
Temperature screening and the role of $E_r$ in neoclassical transport

The radial impurity flux can be written in the form

$$\langle \Gamma_z \cdot \nabla r \rangle = L_{11}^{zz} A_{1z} + L_{11}^{zi} A_{1i} + L_{12}^{zz} A_{2z} + L_{12}^{zi} A_{2i}$$

where we have defined the “thermodynamic forces” and the collisionality

$$A_{1a} = d(\ln p_a)/dr + (Z_a e/T_a) \ d\Phi/dr$$

$$A_{2a} = d(\ln T_a)/dr$$

(note: $T_z = T_i$)

In a tokamak $E_r = -d\Phi/dr$ has no effect on radial neoclassical transport.
Temperature screening of the impurities by the bulk ion temperature gradient can arise.

$$\langle \Gamma_i \cdot \nabla r \rangle \simeq -Z \langle \Gamma_z \cdot \nabla r \rangle$$

In a stellarator $E_r$ has a strong impact on the radial transport.
$E_r$ determined from ambipolarity.
Temperature screening and the role of $E_r$ in neoclassical transport

Conventional wisdom in stellarators (from pitch-angle scattering models)

Intra-species terms $(L_{11}^{zz}, L_{12}^{zz})$ dominate over inter-species terms $(L_{11}^{zi}, L_{12}^{zi})$, i.e.

$$\langle \Gamma_z \cdot \nabla r \rangle \approx L_{11}^{zz}d(\ln p_z)/dr + L_{11}^{zz}(Ze/T_z)d\Phi/dr + L_{12}^{zz}d(\ln T_z)/dr .$$

In ion root $E_r$ is determined by ambipolarity from bulk-ion transport:

$$(e/T_i) \frac{d\Phi}{dr} = - \frac{d(\ln p_i)}{dr} - \left( \frac{L_{12}^{ii}}{L_{11}^{ii}} \right) \frac{d(\ln T_i)}{dr} .$$

Substitute into impurity transport equation

$$\langle \Gamma_z \cdot \nabla r \rangle = L_{11}^{zz}d(\ln p_z)/dr - Z \left\{ d(\ln p_i)/dr + \left( \frac{L_{12}^{ii}}{L_{11}^{ii}} \right) \frac{d(\ln T_i)}{dr} \right\}$$

$$+ L_{12}^{zz} \frac{d(\ln T_z)}{dr} .$$

Coefficient in front of $d(\ln T_i)/dr$:

$$-Z L_{11}^{zz} \left( 1 + \frac{L_{12}^{ii}}{L_{11}^{ii}} \right)$$

is always positive $\Rightarrow$

No temperature screening.
The conventional picture successful in explaining experimental observations, with some notable exceptions:

- The carbon impurity hole in Large Helical Device. [Ida et al., Phys. Plasmas (2009)]

Recent years a revived interest in neoclassical impurity physics, advances in analytical and numerical modeling:

- In Pfirsch-Schlüter regime \( \nu_{zii} = \nu_{zi} / \omega_{ti} \sim \nu_{zi} / v_{Ti} \gg 1 \) (all ion species) the impurity transport is independent of \( E_r \). [Braun, Helander, PoP (2010)]
- Experimentally relevant Mixed-collisionality transport regime, \( \nu_{zzz} \gg 1; \nu_{zii} \ll 1 \), weak drive of impurity transport by \( E_r \), screening from \( \nabla T_i \) possible also in stellarators. [Helander et al., Phys. Rev. Lett. (2017)]
- Effect of flux-surface potential variations \( \Phi_1(\theta, \zeta) = \Phi - \langle \Phi \rangle \). [García-Regaña et al., PPCF (2013); Nucl. Fusion (2017); PPCF (2018)], [Mollén et al., PPCF (2018)], [Buller et al., J. Plasma Phys. (2018)]
- \( \Phi_1 + \) tangential magnetic drifts. [Velasco et al., PPCF (2018)], [Calvo et al., PPCF (2017); arXiv (2018)]

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Numerical tools for calculating neoclassical transport in stellarators

► **DKES** [Hirshman et al., Phys. Fluids (1986)] (Drift Kinetic Equation Solver)

- The main workhorse for neoclassical calculations in stellarators.
- Radially local; mono-energetic, speed is a parameter ⇒ 3D.
- Pitch-angle scattering (momentum correction can be applied afterwards).

New codes start to explore extended physics (these are a few of them):

- **FORTEC-3D** [Satake et al., Plasma Fusion Res. (2008)]
  5D, radial coupling is retained.

- **EUTERPE** [García-Regaña et al., PPCF (2013); Nucl. Fusion (2017)]
  Radially local particle in cell Monte Carlo code. Pitch-angle scattering + momentum correction.
  Flux surface variations of electrostatic potential $\Phi_1 (\theta, \zeta) = \Phi - \langle \Phi \rangle$.

- **SFINCS** [Landreman et al., Phys. Plasmas (2014), Mollén et al., PPCF (2018)]
  Radially local 4D, continuum code. Eulerian uniform grid in $\theta, \zeta$.
  Linearized Fokker-Planck collisions + $\Phi_1$ + additional effects.

- **KNOSOS** [Velasco et al., PPCF (2018)]
  Orbit-averaged equation. Pitch-angle scattering. $\Phi_1$ + tangential magnetic drifts.
Stellarator Fokker-Planck Iterative Neoclassical Conservative Solver

Solves the time-independent radially local $\delta f$ 4D drift-kinetic equation and calculates flows and radial fluxes, e.g.

$$\langle \Gamma_s \cdot \nabla r \rangle = \langle \int d^3v f_1(s)(v_d + v_E) \cdot \nabla r \rangle.$$ 

SFINCS can simultaneously take into account:

- Full linearized Fokker-Planck collision operator.
- Arbitrary number of kinetic species (non-trace impurities, non-adiabatic electrons).
- Self-consistent calculation of ambipolar $E_r$

found by iterating until $\langle \mathbf{J} \cdot \nabla r \rangle = \sum_s Z_s e \langle \Gamma_s \cdot \nabla r \rangle = 0$.

- Flux-surface potential variations

$$\Phi_1(\theta, \zeta) = \Phi - \Phi_0(r); \; \Phi_0(r) = \langle \Phi \rangle; \; \Phi_1 \ll \Phi_0$$

$f_1(s, \theta, \zeta, \xi, x), \Phi_1(\theta, \zeta)$ unknowns

⇒ nonlinear system of equations.

SFINCS available on: [Landreman, Smith, Mollén & Helander, Phys. Plasmas (2014)]

https://github.com/landreman/sfincs
Drift-kinetic equation that SFINCS solves

\[
\begin{aligned}
\dot{R} &= v_\parallel b - (\nabla \Phi_0 \times b)/B \\
\dot{v}_\parallel &= - Z_s e b \cdot \nabla \Phi_1 / m_s - \mu b \cdot \nabla B - v_\parallel (b \times \nabla B) \cdot \nabla \Phi_0 / B^2 \\
\dot{\mu} &= 0 \\
f_{0s} &= f_{Ms} \exp(-Z_s e \Phi_1 / T_s)
\end{aligned}
\]

\[
\begin{aligned}
\dot{R} \cdot \nabla f_{1s} + \dot{v}_\parallel (\partial f_{1s} / \partial v_\parallel) - C_{\text{linear}}[f_{1s}] = \\
= - f_{0s} \left[ n_s^{-1} \, dn_s / dr + Z_s e T_s^{-1} \, d\Phi_0 / dr + (m_s v^2 / 2T_s - 3/2 + Z_s e T_s^{-1} \Phi_1) \, T_s^{-1} \, dT_s / dr \right] (v_{ds} + v_E) \cdot \nabla r
\end{aligned}
\]
Flux-surface asymmetries in stellarators

- Often neglected in transport calculations because impact on main plasma species is small (and equations more complicated to solve).

- Flux-surface variation of $\Phi$ arises to preserve quasi-neutrality.

  $\Phi_1(\theta, \zeta) = \Phi - \langle \Phi \rangle$

- $\Phi_1$ can have strong impact on high-$Z$ impurity transport

  [García-Regaña et al., Nucl. Fusion (2017)]:
  - radial $\mathbf{E} \times \mathbf{B}$-drift can be of the same size as magnetic drift,
  - modify the boundaries of the trapped particle regions,
  - smaller effect expected in neoclassically optimized stellarators,
  - important for impurity transport in tokamaks (both neoclassical and turbulent). [Angioni et al., Nucl. Fusion (2014)]

- Experimental measurements of asymmetric radiation patterns and flux-surface potential variations (TJ-II) confirm the existence of asymmetries [Pedrosa et al., Nucl. Fusion (2015)].
\[ \begin{align*}
\dot{\mathbf{R}} &= v_{\parallel}\mathbf{b} - (\nabla \Phi_0 \times \mathbf{b})/B + \mathbf{v}_{ds} \cdot \nabla f_{1s} \\
\dot{v}_{\parallel} &= -Z_seb \cdot \nabla \Phi_1/m_s - \mu b \cdot \nabla B - v_{\parallel}(b \times \nabla B) \cdot \nabla \Phi_0/B^2
\end{align*} \]

\[ \begin{align*}
\dot{R} \cdot \nabla f_{1s} + \dot{v}_{\parallel}(\partial f_{1s}/\partial v_{\parallel}) - C_{\text{linear}}[f_{1s}] &= \\
&= -f_{0s}[n_s^{-1} dn_s/dr + Z_s e T_s^{-1} d\Phi_0/dr + \\
&+ (m_s v^2/2 T_s - 3/2 + Z_s e T_s^{-1} \Phi_1) T_s^{-1} dT_s/dr](\mathbf{v}_{ds} + \mathbf{v}_E) \cdot \nabla r
\end{align*} \]

- Magnetic drifts implemented in SFINCS [Paul et al., Nucl. Fusion (2017)].
- To include tangential magnetic drifts in a numerical solver is somewhat ambiguous.
  
  Example: Approximation \( df_{1s}/dr = 0 \) in \( \mathbf{v}_{ds} \cdot \nabla f_{1s} \) different in different coordinate systems.
- 9 different versions implemented in SFINCS.
- SFINCS calculations with \( \Phi_1 \) + tangential magnetic drifts very numerically challenging.
- KNOSOS significantly faster. → See talk by J. L. Velasco [Velasco et al., PPCF (2018)]
- Pitch-angle scattering collisions (no momentum correction).
- Large Helical Device equilibrium (10-fold symmetry in $\zeta$) [García-Regaña et al., Nucl. Fusion (2017)].

![Graph and plots showing comparisons between different plasma simulation codes.](image-url)
Benchmark EUTERPE, SFINCS, KNOSOS

- Pitch-angle scattering collisions (no momentum correction).
- TJ-II equilibrium (4-fold symmetry in $\zeta$).
- Pitch-angle scattering collisions (no momentum correction).
- Large Helical Device equilibrium.
- Tangential magnetic drifts.

**Without tangential magnetic drifts**

**With tangential magnetic drifts**
Summary benchmark

► Three different numerical tools EUTERPE, SFINCS, KNOSOS, based on different numerical techniques, used to calculate radial impurity transport and variation of the electrostatic potential $\Phi_1(\theta, \zeta)$ in various stellarator plasmas.

► Benchmark for TJ-II, Large Helical Device and Wendelstein 7-X.

► In about half of the cases studied the agreement between the codes is very good.

► For the other cases there are discrepancies, but the shape of $\Phi_1(\theta, \zeta)$ is always similar. Discrepancy does not seem to be connected to which device is analyzed.

► Study more experimental plasmas, e.g. W7-X OP1.2, and search for the reason to the discrepancy.
Classical impurity transport in stellarators

[Buller et al., J. Plasma Phys. (2018)]

- The flux-surface averaged collisional impurity flux is given by

\[ Z e \langle \Gamma_z \cdot \nabla r \rangle = \langle B \times \nabla r \cdot R_z / B^2 \rangle + Z e \langle n_z B \times \nabla r \cdot E / B^2 \rangle - \langle B \times \nabla r \cdot \nabla p_z / B^2 \rangle. \]

- Classical flux is often neglected as small compared to the neoclassical

\[ Z e \langle \Gamma_z \cdot \nabla r \rangle_{\text{classical}} = (m_i n_i T_i / e n_z \tau_{iz}) \langle n_z |\nabla r|^2 / B^2 \rangle \left[ n_i^{-1} dn_i / dr - 0.5 \cdot T_i^{-1} dT_i / dr \right]. \]

Estimate: \( \langle \Gamma_z \cdot \nabla r \rangle_{\text{classical}} / \langle \Gamma_z \cdot \nabla r \rangle_{\text{neoclassical}} \approx \langle |\nabla r|^2 / B^2 \rangle \langle B^2 \rangle / (\langle u^2 B^2 \rangle \langle B^2 \rangle - \langle u B^2 \rangle^2). \)

- Ratio small for conventional tokamaks/stellarators.

\( u = j_\parallel / (B p') \)

W7-X standard configuration: \( \sim 3.0 - 3.5 \) (optimized for low \( j_\parallel / j_\perp \)).
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Is impurity transport neoclassical in optimized stellarators?

- Wendelstein 7-X OP1.1 discharge 160310028@0.23s x-ray imaging crystal spectrometer (XICS).

- Wendelstein 7-X OP1.2a:
  Iron atoms injected via laser blow-off and analyzed by VUV and x-ray spectrometers.
  STRAHL + DKES modelling of helium plasma #17110918.
  “The anomalous diffusion profile is more than two orders of magnitude larger than the neoclassical one”. [Geiger et al., submitted Nucl. Fusion (2018)]

- Nonlinear gyrokinetic flux-tube simulations of impurity hole plasmas in Large Helical Device with the GKV code find an order of magnitude larger C^{6+}-fluxes than neoclassical calculations. [M. Nunami, M. Nakata]

- Idea: include $\Phi_1$ in linear gyrokinetics. Model based on [Helander, Zocco, PPCF (2018)].
Effect of $\Phi_1$ on quasilinear impurity fluxes

- Non-fluctuating potential
  $$\Phi_1(\theta, \zeta) = \Phi - \Phi_0(r); \quad \Phi_0(r) = \langle \Phi \rangle; \quad \Phi_1 \ll \Phi_0$$

- Energy is
  $$\varepsilon = m_s v^2/2 + Z_s e \Phi_1(\theta, \zeta) + Z_s e \phi(t, \theta, \zeta)$$

  $\Phi_1(\theta, \zeta)$ - equilibrium potential

  $\phi(t, \theta, \zeta)$ - fluctuating potential

**Note:** Keeping $\Phi_0$ in our treatment we will simply find that in linear gyrokinetics it can be transformed away since turbulent transport is automatically ambipolar to lowest order and independent of $E_r = -d\Phi_0/dr$.

- Lowest order distribution
  $$f_{0s} = f_{Ms} \exp(-Z_s e \Phi_1/T_s)$$

  $$f_{Ms} = n_{0s}(\psi) \left( m_s v^2/2\pi T_s \right)^{3/2} \exp(-m_s v^2/2T_s)$$

- $\Phi_1(\theta, \zeta)$ is obtained from a neoclassical calculation with a code like SFINCS. In our gyrokinetic model $\Phi_1(\theta, \zeta)$ is an input.
Effect of $\Phi_1$ on quasilinear impurity fluxes

- Linear gyrokinetic equation for the non-adiabatic distribution $g_s$

$$f_s = f_{0s} \left(1 - Z_s e \phi/T_s\right) + g_s$$

$$v_\parallel \nabla_\parallel g_s - i \left(\omega - \omega_E - \omega_{ds}\right) g_s = C[g_s] - i \left(Z_s e \phi/T_s\right) J_0(k_\perp v_\perp/\Omega_s) f_{0s} \left(\omega - \omega_{*s}\right)$$

$$\omega = \omega_r + i\gamma$$

$$\alpha = q(\psi) \theta - \zeta$$

$$k_\perp = k_\alpha \nabla \alpha + k_\psi \nabla \psi \approx k_\alpha \nabla \alpha$$

$$\omega_E = v_{\Phi_1} \cdot k_\perp = (k_\alpha/B) \left(b \times \nabla \Phi_1\right) \cdot \nabla \alpha$$

(usually ignored because small for $i, e$)

$$\omega_{ds} = v_{ds} \cdot k_\perp = k_\alpha \left[b \times (v_\perp^2 \nabla \ln B/2 + v_\parallel^2 \kappa)/\Omega_s\right] \cdot \nabla \alpha$$

$$\omega_{*s} = - (T_s/Z_s e B) f_{0s}^{-1} \left(b \times k_\perp\right) \cdot \nabla (f_{0s})_\varepsilon = \omega_{*s} q \left[1 + \eta_s (m_s v^2/2T_s - 3/2 + Z_s e T_s^{-1} \Phi_1)\right]$$

$$\omega_{*s} = (k_\alpha T_s/Z_s e) d \ln n_{0s}/d\psi; \quad \eta_s = (d \ln T_s/d\psi) / (d \ln n_{0s}/d\psi)$$

We neglect parallel streaming $v_\parallel \nabla_\parallel g_s$ and collisions $C[g_s]$. 
Effect of $\Phi_1$ on quasilinear impurity fluxes

- The $E \times B$ drift frequency $\omega_E$ usually neglected because it is small, unless $Z_s e \Phi_1 / T_s \sim O(1)$.

- Note that $\omega_E$ independent of $Z_s$, whereas

  $\omega_{ds} \sim 1/Z_s$

  $\omega^T_{\times s} \sim 1/Z_s$.

  $\Rightarrow$ for high-$Z$ impurities $\omega_E$ could play a role.

- The flux-surface-averaged quasilinear impurity flux is given by

  $$\Gamma_z = - k_\alpha \text{Im} \left[ \langle \int g_z J_0 \phi^* \ d^3v \rangle \right]$$

  and we find that

  $$\Gamma_z = - (Ze/T_z) \ k_\alpha \gamma \ \langle |\phi|^2 \int (\omega^T_{\times z} - \omega_E - \omega_{dz}) \ |\omega - \omega_E - \omega_{Dz}|^{-2} \ J_0^2 \ f_{0z} \ d^3v \rangle$$

  which implies that $\Phi_1$ can only change the sign of $\Gamma_z$ if it can change the sign of

  $(\omega^T_{\times z} - \omega_E - \omega_{dz})$. 
To perform the velocity integral we assume:

- Low-\(\beta\) plasma \(\Rightarrow\) simplify \(\omega_dz\) using \(\kappa \approx \nabla_\perp B / B\):
  \[
  \omega_dz = \omega_B \left( \frac{v_\perp^2}{2} + v_z^2 \right) / v_z^2
  \]

- Ion-scale turbulence \(\Rightarrow\) \(k_\perp^2 \rho_z^2 / 2 \ll 1\).

- Assume high-\(Z\) trace impurities so \(\omega\) obtained from bulk species gyrokinetic equation.

- Order \(\omega_E / \omega, \omega_dz / \omega, \omega_{T_{xz}} / \omega\) and \(J_0(k_\perp v_\perp / \Omega_z) - 1\) as \(1/Z\) small quantities.

Use Boozer coordinates \(B = H(\psi, \theta, \zeta) \nabla \psi + I(\psi) \nabla \theta + G(\psi) \nabla \zeta\).

\[
\Gamma_z \simeq - (Ze / T_z) k_\alpha \left[ \frac{\gamma}{(\omega_r^2 + \gamma^2)} \right] n_{0z}(\psi) \ q \ \omega_{xz} \ \langle |\phi|^2 \exp(-Z_se\Phi_1 / T_s) \ \{1 + \eta_z \ ZeT_z^{-1} \Phi_1 - \omega_E / (q \ \omega_{xz}) - \omega_B / (q \ \omega_{xz}) \} \right] =
- k_\alpha^2 \left[ \frac{\gamma}{(\omega_r^2 + \gamma^2)} \right] (dn_{0z} / d\psi) \ q \ \langle |\phi|^2 \exp(-Z_se\Phi_1 / T_s) \ \{1 + \eta_z \ ZeT_z^{-1} \Phi_1 \} + (Ze / T_z) (dlnn_{0z} / d\psi)^{-1} (q \ G + I)^{-1} [H (q \ d\Phi_1 / d\zeta + d\Phi_1 / d\theta) + \theta \ dq / d\psi (Gd\Phi_1 / d\theta - Id\Phi_1 / d\zeta)] + (2 / B) (dlnn_{0z} / d\psi)^{-1} (q \ G + I)^{-1} [H (q \ dB / d\zeta + dB / d\theta) + \theta \ dq / d\psi (GdB / d\theta - IdB / d\zeta)] - (2 / B) (dlnn_{0z} / d\psi)^{-1} dB / d\psi \} \]

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Effect of $\Phi_1$ on quasilinear impurity fluxes

- Using $B = H(\psi, \theta, \zeta) \nabla \psi + I(\psi) \nabla \theta + G(\psi) \nabla \zeta$ with
  
  $G \gg I$ (poloidal current outside flux-surface $\gg$ toroidal current inside flux-surface).

  $|H \nabla \psi|/(G|\nabla \psi|) \sim (\beta \Delta B/B)/(r/R_0) \ll 1 \Rightarrow$ neglect $H/G$ terms.

\[
\Gamma_z \approx- k_x^2 [\gamma/(\omega_r^2 + \gamma^2)] \left( \frac{dn_{0z}}{d\psi} \right) q \left\langle \phi \right\rangle^2 \exp\left(-Z_s e \Phi_1/T_s\right) \{1 + \eta_z ZeT_z^{-1} \Phi_1 \}
\]

\[
+ (d\ln n_{0z}/d\psi)^{-1} \theta q^1 dq/d\psi \left(Ze/T_z\right) d\Phi_1/d\theta
\]

\[
+ (2/B) (d\ln n_{0z}/d\psi)^{-1} \theta q^1 dq/d\psi dB/d\theta - (2/B) (d\ln n_{0z}/d\psi)^{-1} dB/d\psi\}.
\]

- What is the physics behind the $\eta_z ZeT_z^{-1} \Phi_1$ term?

Real lowest-order density $N_{0z}(\psi, \theta, \zeta) = n_{0z}(\psi) \exp(-Z_s e \Phi_1/T_s) \Rightarrow$

\[
d\ln N_{0z}/d\psi = (d\ln n_{0z}(\psi)/d\psi) \left(1 + \eta_z ZeT_z^{-1} \Phi_1 \right)
\]

varies over the flux-surface with $\Phi_1$.

- The most important is $d\ln N_{0z}/d\psi$ where the turbulence is located!

- Remains to explore size of other terms in $\Gamma_z$. 

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The impurity hole in the Large Helical Device

- No accumulation of C\textsuperscript{6+} impurities in Large Helical Device although all predictions of both neoclassical and turbulent transport point towards accumulation. (Inward pointing $E_r$).


Assuming that external source/sink is zero (or negligible) steady density profiles should be sustained by balanced fluxes:
\[ \Gamma_c^{(turb)} + \Gamma_c^{(neo)} = 0 \]

- Still an open problem.

- Large Helical Device deuterium experiment started March 2017.

C\textsuperscript{6+} profile more peaked in deuterium plasmas than in hydrogen plasmas.

[Morisaki et al., International Stellarator-Heliotron Workshop (2017)]

Isotope effect on C\textsuperscript{6+} transport. \textit{Suggests that turbulent impurity transport dominates?}
\( \Phi_1 \) in neoclassical transport does not seem to explain the impurity hole in LHD

- Neoclassical particle fluxes compared to turbulent particle fluxes at steady-state.
- Direction of \( e^- \), \( H^+ \) and \( \text{He}^{2+} \)-fluxes match; \( \text{C}^{6+} \)-fluxes do not match!
- Can \( \Phi_1 \) in neoclassical calculation explain the discrepancy in the \( \text{C}^{6+} \)-fluxes?
- **SFINCS calculations:**
  - \( \Phi_1 \) can vary strongly on flux-surface: \( \pm 200 \, \text{V} \).
  - \( \Phi_1 \) has large impact on \( \text{C}^{6+} \)-fluxes, but in wrong direction to explain hollow \( \text{C}^{6+} \)-profile.
Can effect of $\Phi_1$ on quasilinear impurity fluxes explain the impurity hole in LHD?

Large Helical Device
10-periodic in toroidal direction

Bad curvature $L2$

Metric coefficient $g^{11} = |\nabla \psi|^2$

- Most probable location for turbulence is areas on outboard side between ridges (around $\theta = 0, \zeta = 0$). There $L2 < 0$ (bad curvature) and $g^{11}$ is maximized $\Rightarrow$ optimal conditions for turbulence.
- Approximate $|\phi|^2$ with 2D parabola around $\theta = 0, \zeta = 0$. 
Can effect of $\Phi_1$ on quasilinear impurity fluxes explain the impurity hole in LHD?

- Large Helical Device discharge 113208 at $t = 4.64s$

![Graph showing densities and temperatures](image)

- Look at $r/a = 0.7$, hollow density profile,

  $$
  \eta_z = \frac{d \ln T_z/d\psi}{d \ln n_0z/d\psi} = -3.5,
  \quad
  \Phi_1(0, 0) = 34.5 \text{ V},
  \quad
  \eta_z \, Z e T_z^{-1} \Phi_1(0, 0) = -0.29.
  $$

- $\eta_z \, Z e T_z^{-1} \Phi_1$ seems to contribute to outward $\Gamma_z$.

- Maybe not enough to explain impurity hole but a more careful analysis is needed.
Notes on quasilinear impurity fluxes

Effect of $\Phi_1$ could possibly become stronger by:

- Tangential magnetic drifts included in the SFINCS calculations.

- Including effects of plasma heating.

- Include parallel streaming term.
  Axi-symmetry: Trapped Electron Modes $\Rightarrow$ outwards transport,
               Ion Temperature Gradient modes $\Rightarrow$ inwards transport.

- Including radial variation $\Phi_1(\psi, \theta, \zeta)$, requires radially global neoclassical code.
Outline

- Introduction to impurity transport in stellarators
- Neoclassical calculations with equilibrium electrostatic potential variations $\Phi_1$
- $\Phi_1$ in linear gyrokinetic modelling
- Summary
Summary

- Three different numerical tools EUTERPE, SFINCS, KNOSOS that can calculate $\Phi_1$ have been benchmarked to each other. In several cases the agreement is very good, but some discrepancies have to be solved.

- $\Phi_1$ could play a role in quasilinear impurity transport, but work remains to explore this effect further. Linear gyrokinetic flux-surface simulations?
Extra slides
SFINCS implementation and numerical details

- Eulerian uniform grid in $\theta$, $\zeta$
  MPI parallelization with PETSc library + MUMPS

- Spectral discretization in $\xi = \frac{v_\parallel}{v}$: Legendre polynomials $P_n(\xi)$

- Spectral collocation discretization for $x = \frac{v}{v_{Ts}}$, non-standard orthogonal polynomials
  Collocation: function is known on a set of grid points rather than explicitly
  expanded in a set of modes $\Rightarrow$ integration/differentiation weight matrices.

- Non-linear system solved with Newton method:
  $x = (f_1, \Phi_1)$
  Residual $R(x) = 0$
  Jacobian $R' = \frac{\delta R(x)}{\delta x}$
  State-vector updated as $x_{n+1} = x_n - \frac{R(x_n)}{R'(x_n)}$

- System solved using preconditioned GMRES.

- Code written in Fortran (also MATLAB version).
SFINCS numerical resolution, expensive simulations at low collisionality

- Trapped-passing boundary (tokamak example):

- Simulations typically become more demanding at low collisionality (small $\nu_{ss}/\nu_{Ts}$). Thinner trapped-passing boundary layer harder to resolve.

- Resolution in SFINCS runs for W7-X OP1.1:
  \[(N_{\text{species}} \times N_{\theta} \times N_{\zeta} \times N_{x} \times N_{\xi}) \times (N_{\text{species}} \times N_{\theta} \times N_{\zeta} \times N_{x} \times N_{\xi}) \sim 10^7 \times 10^7\]
  Runs on IPP Draco cluster $\leq 32$ nodes (128GB) in $\leq 20$ min (often $\leq 5$ min)

- Most time consuming activities:
  - find numerical convergence
  - find ambipolar $E_r$
Flux-surface potential variations $\Phi_1$ in collision operator

$$C_{ab}^{\text{linear}}[f_s] = C_{ab}[f_{Ma}, f_{Mb}] \exp(-Z_a e \Phi_1 / T_a - Z_b e \Phi_1 / T_b) +$$

$$+ C_{ab}[f_{1a}, f_{Mb}] \exp(-Z_b e \Phi_1 / T_b) + C_{ab}[f_{Ma}, f_{1b}] \exp(-Z_a e \Phi_1 / T_a)$$
Multigrid version of SFINCS

[Landreman APS 2017]

► In neoclassical transport calculations high resolution is required in at least 3 dimensions (poloidal angle $\theta$, toroidal angle $\zeta$, pitch-angle $\xi$) due to internal boundary layers.

► Continuum solvers often use a direct solver, which scales poorly with resolution.

► 3D **multigrid** version of SFINCS (mono-energetic: velocity $x$ input parameter).

**Geometric multigrid (there is also Algebraic multigrid):**

► Gauss-Seidel iterative method quickly reduces short-wavelength errors but is ineffective for long-wavelength errors. On coarser grid, long-wavelength errors are more quickly corrected.

► V-cycle: Combination of Gauss-Seidel smoothing with a coarse-grid solve.

  Coarse-grid solve recursively.

  On coarsest level, a direct solve is cheap.

► Test case on IPP computer Draco:
  - DKES gets radial transport to +/- 12% in 58 160s (1 proc).
  - Algebraic multigrid code +/- 4% in 168s (1 proc) or 33s (32 procs).