Impurity transport modelling in tokamaks
Recent progress

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Thanks to C. Angioni, T. Fülöp, S. Futatani, C. Giroud, A. Skyman, P. Strand, M. Valisa
Outline

• Background and motivation
• Impurity particle transport driven by ITG/TE modes
• Recent results on impurity transport modelling in core tokamak plasmas:
  - fluid and gyrokinetic models
    - quasilinear and nonlinear turbulence simulations
    - comparisons with experimental data
• Summary
Background and motivation

- Radiating boundary beneficial but impurity accumulation in core can be detrimental:
  - What determines the impurity density profile?
  - Will impurities accumulate in the center?
  - Control of accumulation by central heating?
  - Scaling of transport with impurity charge and mass?
- Anomalous transport usually dominates neoclassical transport in confinement region.
- ITG/TE mode transport paradigm.
Impurity transport

- Impurity particle flux:
  \[ \Gamma_{nz} = \langle \delta v_E \delta n_z \rangle = -D_z \nabla n_z + n_z V_z \]

- Diffusion \( D_z \) and convective velocity \( V_z \) (pinch) independent of \( \nabla n_z \) for trace levels of impurities.

- Zero-flux condition \( \Gamma_{nz} = 0 \) gives normalised peaking factor
  \[ \text{PF} = \frac{R}{L_{nz}} = -\frac{R \nabla n_z}{n_z} = -\frac{R V_z}{D_z}. \]

  \( \text{PF}>0 \) for peaked profiles
  \( \text{PF}<0 \) for hollow profiles

- Three pinch terms identified using QL theory (neglecting rotation effects) [Angioni PRL 2006, Dubuit PoP 2007]:
  \[ \Gamma_{nz} = -D_z \left\{ \nabla n_z - C \nabla T_z \left( \omega \frac{T_z}{T_z} n_z + C_{\text{curv}}(s) \frac{1}{R} n_z + C_{\text{vis}}(\omega) n_z \right) \right\} \]

  - **Thermodiffusion**
  - **Curvature pinch**
  - **Parallel compressibility**
Impurity transport

• Properties of pinch terms:

<table>
<thead>
<tr>
<th></th>
<th>Compression</th>
<th>Direction</th>
<th>Charge/mass dep.</th>
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<tbody>
<tr>
<td>$V_Z$</td>
<td>div($v_{ExB}$)</td>
<td>Inward*</td>
<td>Independent</td>
</tr>
<tr>
<td>Curvature pinch</td>
<td>div($n_Z v_{Z,*}$)</td>
<td>Inward (TEM)*</td>
<td>$1/Z$</td>
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<td></td>
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<td>Outward (ITG)*</td>
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<tr>
<td>Thermodiffusion</td>
<td>div($n_Z v_{Z}$)</td>
<td>Inward (ITG)</td>
<td>Z/A</td>
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<tr>
<td>Parallel compress.</td>
<td>div($n_Z v_{Z</td>
<td></td>
<td>}$)</td>
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</tbody>
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* May reverse sign for negative shear. [Dubuit PoP 2007, Bourdelle PoP 2007, Futatani PRL 2010]

• Toroidal rotation (Coriolis force, centrifugal force and rotation gradient $u'$) introduce additional terms, $\Gamma_{nz} \sim C_u u'$ [Camenen PoP 2009]

• Electromagnetic effects [Hein and Angioni PoP 2010, Hein this mtg O3.02]
Modelling of impurity transport at JET

- Interpretative analysis and predictive modelling of impurity injection experiments* at JET:
  - Ne, Ar, Ni injected.
  - $D_Z$ and $V_Z$ determined experimentally (and PF for C).

- Anomalous transport model comparison:
  - Weiland fluid model for ITG/TE modes.
  - Quasilinear and nonlinear GK fluxtube simulations with GENE.

- Electrostatic, collisionless plasma, simple s-$\alpha$ equilibrium.

- Trace levels of impurities ($n_Z/n_e<10^{-3}$).

Model comparison: Z scaling

- Peaking factor PF vs Z at mid radius for ITG dominated discharge.
- Weiland model, QL and NL GK fluxtube simulations.
- Good agreement between fluid and NL GK results for Ne, Ar, Ni.
- Simple fluid limit give PF=2 for large Z (without parallel compression).
- Z-scaling from thermopinch.
- Moderate values of PF (<< neoclassical prediction).
- \( D_{\text{He}} / \chi_i \approx 1 \) (fluid, NL GENE).

\[ \text{Peaking factor vs } Z, \ Z \geq 2 \ (A_Z=2Z). \]

The parameters are \( I=1.8 \text{MA}, \ B_T=3 \text{T}, \ P_{\text{NBI}}=4.2 \text{MW} \): \( R/L_{ne}=2.7, \ R/L_{Tj}=5.6, \ T_e/T_i=1, \ q=2.4, \ s=0.6. \)

[Nordman EPS 2010]
Comparison with experiment

Fig. Radial profiles of (a) $D_Z$ ($m^2/s$) and (b) $V_Z$ ($m/s$) for Ne, Ar and Ni, discharge #67730, #67732 and Weiland model ($k_\theta \rho=0.2$).

- Reasonable agreement for Ne, Ar, Ni at mid radius: $D_Z$ weakly dependent on $Z$, inward pinch $V_Z$. NC subdominant.

- Main discrepancy: experimental C profile flat or hollow ($PF_{Cexp} \approx 0$, [Weisen NF 05, Giroud IAEA 06]), theory gives $PF_C = 1.9$ (fluid) and $PF_C = 1.7$ (NL GENE).

[Nordman et al, EPS 2010]
Carbon peaking discrepancy

- Some possible explanations examined:
  - Validity of trace results for experimental levels of C (2%)?
  - Effects of ExB shearing (using Waltz rule)? Effective reduction of ITG growth rate => reduced peaking factor for low Z - not significant here with $\gamma_E/\gamma_I \approx 0.1$.
  - Effects of collisions - not significant.
  - Predictive simulations including impurity transport.

- Missing ingredient in models?

[Nordman et al, EPS 2010]

Peaking factor $PF$ versus $Zf_c=$$Zn_Z/n_e$ (a) and versus $\gamma_E/\gamma_I$, (b) at $r/a\approx 0.5$. 
Predictive simulations

- Predictive JETTO/SANCO simulations of $T_i = T_Z$, $T_e$, $n_e$, and $n_Z$.
- ITG/TE transport (Weiland fluid) and NC transport.
- PF for C consistent with interpret results: $PF_C = 1.8$ in predictive sim vs $PF_C = 1.9$ in interpret sim.
- For $\rho < 0.2$ (and for $Z = 28$) strong peaking is obtained due to neoclassical transport (not seen in exp).

[Nordman et al, EPS 2010]
Impurity transport in TEM regime

• PF vs Z in TEM regime.
• Weiland model and QL GENE simulations in trace impurity limit (collisionless).
• Reversal of thermopinch and parallel compression pinch as compared to ITG case.
• PF decreases with Z: $\text{PF}_{\text{TEM}} < \text{PF}_{\text{ITG}}$ for large Z.

[Skyman et al., EPS 2010]

Peaking factor vs Z, $Z \geq 2$ ($A_Z=2Z$). The parameters are $R/L_{T_e}=7$, $R/L_{T_{T_i,Z}}=3$, $R/L_{n_e}=3$, $T_e/T_i=1$, $s=0.8$, $q=1.4$. 
Impurity control with RF heating

- Peaked Ni profile in ion heated regime [58144, ITG dominated (GS2)]
- Hollow Ni profile with dominant electron heating [58143, TEM dominated] [Puiatti PoP 2006]
- Qualitative agreement with theory (reduction of PF with transition from ITG to TEM turbulence), but no flux reversal obtained.

[Puiatti, this mtg O3.01]

Fig. Steady state Ni profiles, calculated from exp $V_z$ and $D_z$
Analytical transport model

• Semi-analytical kinetic model for ITG driven impurity transport.
• Based on boundary layer solution for the gyrokinetic equation assuming:
  - large-aspect-ratio, circular cross section, toroidal symmetry, weakly collisional plasma
  - model electrostatic potential: \( \phi(\theta) = \phi_0 \left( \frac{1 + \cos(\theta)}{2} + i f_s \sin^2(\theta) \right) \)
    , \( f_s = -0.6s + s^2 - 0.3s^3 \)
• Analytical expressions, without expansion in the smallness of the magnetic drift frequencies.
• Eigenvalues and impurity particle fluxes agree well with gyrokinetic calculations using GYRO (parallel dynamics neglected).

[Fülöp et al., PoP 2010]
Impurity peaking factor

- Analytical expression for the impurity peaking factor derived from $\Gamma_Z=0$, no trace assumption.

\[
\frac{R}{L_{nz}} = \frac{2+3s}{2} \left( 1 - \frac{2}{1+\gamma^2} \frac{k_\theta \rho_s}{Z \tau_z \omega_0} \left( \frac{R}{L_{TZ}} - \frac{5(2+3s)}{6} \right) \right)
\]

- Balance between curvature pinch and diffusion gives
  \[\frac{R}{L_{nz}}=2<\omega_{DZ}(\theta)/\omega_{DZ}(0)>=(2+3s)/2.\]

- Effects of other parameters like $R/L_{ne}$, $T_e/T_i$, collisionality etc enter through $\omega$, $\gamma$ (weak dependence for large $Z$).

Fig. $\Gamma_Z$ vs $a/L_{nz}$ for $Z_{\text{eff}}=1.5$, $Z=6$ (solid), $Z_{\text{eff}}=2$, $Z=6$ (dashed), $Z_{\text{eff}}=2$, $Z=10$ (dotted). Cf between model and QL GYRO (dots and squares). [Fülöp PoP 2010]
Reversed magnetic shear configurations

- Fluid simulation of ITG/TE mode turbulence with global 3D TRB code with monotonic and reversed q.
- Evolution of density, pressure and parallel dynamics for each species (ions, trapped electrons, impurities).
- Impurities are injected in steady state at $r/a=0.8$.

Fig. Radial dependence of $T_i$, $T_e$, $n_i$ from a simulation with monotonic safety factor $q$ (left) and reversed $q$ (right).

[Futatani et al. PRL 2010]
Validation of the diffusion-advection equation

- Trace levels of impurities are injected in a steady turbulent state at \( r/a = 0.8 \).
- The injection of impurities leads to a transient that can be used to determine \( D_z \) and \( V_z \) at each radial position.

\[
\frac{\Gamma}{n} = -D \frac{\nabla n}{n} + V
\]

\( D = 0.47 \)
\( V = -0.13 \)

*Fig. Scatter plot of \( \Gamma_z/n_z \) vs \( \nabla n_z/n_z \) for helium in reversed q profile.*

[Futatani PRL 2010]
Reversal of impurity pinch velocity

- Reversal of pinch direction obtained, from inward (monotonic $q$) to outward (reversed $q$) inside transport barrier due to reversal of the curvature pinch ($\sim<\omega_{DZ}(\theta)>$)

$V<0$: inward direction (accumulation)

$V>0$: outward direction (decontamination)

**Fig.** Radial profile of impurity convective (pinch) velocity $V$ for He: (left) w/o transport barrier and (right) with transport barrier. [Futatani PRL 2010]
Modelling of Boron transport in AUG

• Modelling of Boron (Z=5) transport in AUG experiments with central ECH in NBI heated H-mode plasmas.

• Turbulent impurity flux obtained by QL gyrokinetic calculations including roto-diffusion $D_{uZ}$ with Coriolis drift (centrifugal effects neglected, $u'_{Z} = R^2 d\Omega_{Z}/dr/\nu_{thZ}$):

$$\frac{R\Gamma_{nZ}}{n_{Z}} = D_{NZ} \frac{R}{L_{nZ}} + D_{ThZ} \frac{R}{L_{TZ}} + [D_{uZ} u'_{Z}] + RV_{pZ}$$

• Roto-diffusion is outward (inward) for ITG modes (TEM) and scales like A/Z.

• ITG dominated discharges, input parameters at r/a=0.5.

• Neoclassical transport negligible at r/a=0.5

[Angioni et al., this mtg P2.13]
Roto-diffusion significant

- Agreement for the NBI heated only phase, roto-diffusion critical ingredient to predict negative values of $R/L_{nB}$ (local hollowness).
- Experimental trend from $R/L_{nB} \leq 0$ with NBI only to $R/L_{nB} > 0$ with high ECH power is reproduced by the modelling.
Summary

- Impurity transport modelling based on fluid and GK simulations (without roto-diffusion):
  - Good agreement between models for Z-scaling of peaking factor in ITG and TEM regimes.
  - Semi-analytical kinetic model in good agreement with GK simulations.
  - Models give reasonable agreement with JET experiments for peaking factors and $V_z, D_z$ (Ne, Ar, Ni).
  - Models fail to explain flat/hollow C profiles in experiments.
  - Inner core transport not well described by models (e.g. impurity pump out by RF heating).
- Roto-diffusion critical ingredient for prediction of hollow Boron profiles in AUG – likely the missing ingredient in transport models.
- Reversal of pinch velocity (from inward to outward) in fluid simulations of reversed magnetic shear configurations in the presence of ITB.