Parametric dependences of impurity transport in neoclassical, reactive drift wave and gyrokinetic descriptions

H. Nordman¹, T. Fülöp¹, J Candy², P. Strand¹ and J. Weiland¹

¹ EURATOM/VR Fusion Association, Dept. of Radio and Space Science, Chalmers University of Technology, Göteborg, Sweden
² General Atomics, San Diego, California

Impurity transport in tokamaks is studied using an electrostatic fluid model for main ion and impurity temperature gradient (ITG) mode and trapped electron (TE) mode driven turbulence and the results are compared with nonlinear gyrokinetic simulations using GYRO and neoclassical theory. Transport scalings with magnetic shear and impurity fraction are investigated, and the validity of the trace impurity approximation is studied. Comparisons between anomalous and neoclassical transport predictions are performed for ITER-like profiles based on ASTRA modelling.

Reactive drift wave model

The reactive drift wave model is based on the solution of a set of fluid equations for the perturbations in density, parallel velocity and pressure for ions, impurities and trapped electrons [1] in the collisionless, electrostatic limit. The closure of the equations is obtained by assuming that the heat flux is equal to the diamagnetic heat flux for all particle species. For the trapped electron model, the electron magnetic drift is, after the bounce averaging, replaced by the precession frequency of trapped electrons as \( \langle \omega_{De} \rangle = \omega_{De} \lambda_t \) with \( \lambda_t = 1/4 + 2s/3 \) [2], where \( s = (r/q)dq/dr \) and \( q \) is the safety factor. We assume adiabatic free electrons and the quasi-linear particle fluxes are computed from \( \Gamma_{n j} = \langle \delta n_j v_{E j} \rangle \), which is summed over all unstable modes for a fixed space scale of the turbulence, with \( (k_r \rho_s)^2 = (k_\theta \rho_s)^2 = 0.1 \), where \( r \) and \( \theta \) are radial and poloidal coordinates. \( \rho_s = c_s/\Omega_{ci} \), \( c_s = \sqrt{T_e/m_i} \) is the sound speed and \( \Omega_{ci} \) is the cyclotron frequency. The eigenvalue equation is reduced to a set of algebraic equations using the semilocal analysis of [3] where the norms \( \langle k_\parallel^2 \rangle, \langle k_\perp^2 \rangle, \langle \omega_{Di,z} \rangle \), with \( \langle \cdots \rangle = \int_0^\pi \int_0^\pi \phi(\cdots) \phi d\theta \), are calculated using a strongly ballooning eigenfunction. The solution of the eigenvalue problem gives the eigenvalues and the perturbations in density, temperature and parallel velocity in terms of the perturbed electrostatic potential. The saturation level of the electrostatic potential is estimated by balancing the linear growth with the dominant convective nonlinearity in the energy and continuity equations. The strong ballooning approximation has recently been shown to give results in good agreement with the results of calculations based on a shear-dependent eigenfunction with general modewidth and with gyrokinetic simulations [4].
Gyrokinetic calculations
We have performed flux-tube (local) simulations with the GYRO code [5]. The transport coefficients are computed including nonlinear gyrokinetic dynamics of both ion species, electron physics was taken to be drift-kinetic. A 128-point velocity-space grid (8 energies, 8 pitch angles and 2 signs of velocity) is used, together with 10 poloidal (orbit) gridpoints per sign of velocity. In the perpendicular directions \((x, y)\), we use a domain size of \((L_x, L_y)/\rho_s = (122, 128)\).

Neoclassical impurity transport
Impurities in high-temperature plasmas, like ITER are expected to be in the banana regime. In this collisionality regime, neoclassical transport is usually outwards due to temperature screening and therefore it has opposite sign to turbulent transport, but is much smaller. It depends on \(q\) but is not sensitive to \(s\). If \(Z\) is large, the neoclassical flux is mainly driven by ion gradients. For moderate or low \(Z\), the flux driven by the impurity gradients will reduce the total impurity flux, since it has opposite sign to the flux driven by the ion gradients.

Trace impurities and dilution model
In the limit of trace impurities, the effect of impurities is neglected in quasi-neutrality condition \((Z f_z \rightarrow 0, \text{where } f_z = n_z/n_e)\), so that the effective diffusivity \(D_z\) does not depend on trace impurity parameters [6, 7]. In the dilution model, the dilution of main ions \((1 - Z f_z)\) is included in quasi-neutrality condition, but the impurity response \(Z f_z \delta n_z/n_z\) is neglected. Figure 1 shows the normalized impurity flux versus \(R/L_{nz}\) in units of \(2\rho_s^2 c_s/R\) for various impurity fractions and \(Z = 6, A_z = 12, q = 1.4, s = 0.5, R/L_{ne} = 3, R/L_{Te} = R/L_{Ti} = R/L_{Tz} = 5, \) where \(L_{nj} = -n_j/n'_j\) and \(L_{Tj} = -T_j/T'_j\) are the density and temperature scale lengths for particle species \(j\). The results of the dilution model (dashed) are compared with the self-consistent model (solid), neglecting the parallel dynamics.

Figure 1. Normalized impurity flux for (black) \(f_z = 0.001\), (red) \(f_z = 0.02\), (blue) \(f_z = 0.05\). The results of the dilution model are the dashed lines and neoclassical transport are the dotted lines. For \(Z = 6\) the trace impurity model gives qualitatively correct results if \(f_z < 0.02\), where \(f_z = n_z/n_e\). The dilution model gives a fair agreement up to \(f_z < 0.05\).
Shear dependence [4]

Figure 2 (left) illustrates the shear dependence of effective diffusivities $D_e$ and $D_z$ for the reactive fluid and gyrokinetic models. In general, the shear dependence of the impurity diffusivity is found to be weaker than that of the electron diffusivity. However, for weak, negative and large positive shear, a strong reduction of the effective impurity diffusivity is obtained. The fluid and gyrokinetic models give qualitatively similar results for the shear scaling of the impurity transport but the fluid diffusivities are typically a factor two lower than the corresponding gyrokinetic diffusivities. This is partly due to the fixed space scale of the turbulence $(k\theta\rho_s)^2 = 0.1$ in the reactive drift wave model. In Figure 2 (right), the shear dependence of $D_z$ for a flat impurity density profile is displayed. As observed, the scaling with $Z$ is very weak for $Z \geq 6$, since here the curvature pinch dominates. For $Z = 2$, the outward thermodiffusive contribution ($\sim 1/Z$) is significant and results in a reduced pinch. The dotted lines show the neoclassical diffusivity (in units of $2\rho_s^2 c_s/R$) for $Z = 2$ (black) and $Z = 6$ (blue).

![Figure 2. Left: Shear scaling of $D_e$ and $D_z$ in units of $2\rho_s^2 c_s/R$ using the reactive drift wave model for $Z = 6$, $A_z = 12$ (blue), $Z = 2$, $A_z = 4$ (black). The other parameters are $R/L_{Te} = R/L_{Ti} = R/L_{Tz} = 9$, $Z f_z = 0.12$, $f_t = 0.5$, $q = 2$, $T_i = T_z = T_e$ and $R/L_{ne} = R/L_{nz} = 3$. Right: Shear scaling of $D_z$ for $R/L_{nz} = 0.1$, $Z = 2$ (black), $Z = 6$ (blue), $Z = 12$ (green), and $Z = 48$ (purple). The triangles are GYRO-results for $Z = 6$. ITER-like plasmas](image)

The selected scenario is a hybrid-mode, with a plasma current of 12 MA, major radius $R = 6.2$ m, minor radius $a = 2$ m, and magnetic field $B = 5.3$ T [8]. The density profile is flat and impurity and ion temperatures are assumed equal. The turbulent impurity flux for $Z = 6$ is calculated using the reactive fluid model in the strong ballooning approximation (including impurity finite-Larmor-radius-effects for completeness) and the results are compared with a local version of the model (with $\lambda_t = 1$, and $k_\perp^2$, $\omega_{Di,z}$ evaluated at $\theta = 0$) which is independent of magnetic shear. Figure 3 shows the impurity diffusivities (left) and electron diffusivities (right) from the reactive fluid model. We note that the results of the shear dependent model differ sig-
significantly from the results of the local analysis. The reason for the sudden change in the fluxes around \( r/a \approx 0.35 \) is that the magnetic shear of the selected ITER-scenario varies from \( s = 0 \) at \( r/a = 0.3 \) to \( s = 0.5 \) at \( r/a = 0.4 \). This change in the shear affects the impurity transport strongly, so that it even reverses its sign. The reason for the large inward pinch at \( r/a = 0.4 \) is that the magnetic shear is close to \( s \approx 0.5 \) where the impurity pinch is strongest, see Fig. 2 (right). As a result of this, the turbulent flux is inward in central part of the plasma but outward in the inner core \( r/a \lesssim 0.3 \) and outside \( r/a \gtrsim 0.7 \). The neoclassical impurity transport is mainly driven by the background ion gradients and is outwards due to temperature screening. The electron transport is inward for the flat ITER density profile but the bounce-averaged TE model predicts significantly weaker transport in the core region where the magnetic shear is weak.

![Figure 3](image_url)

**Figure 3.** Left: Impurity diffusivity for \( Z = 6 \) versus \( r/a \): (black) no magnetic shear dependence, (blue) \( \lambda_t = 1/4 + 2s/3 \), (red) neoclassical. Right: Electron diffusivity versus \( r/a \) [9]: (black) no magnetic shear dependence, (green) \( \lambda_t = 1 \), (blue) \( \lambda_t = 1/4 + 2s/3 \).

**References**


**Acknowledgements** This work was funded by the European Communities under Association Contract between EURATOM and Vetenskapsrådet and US Department of Energy Grant DE-FG03-95ER54309.