Impurity Transport in ITER-like Plasmas

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Abstract Neoclassical impurity transport is compared with transport calculated from the reactive drift wave model of turbulent transport for an ITER-like scenario. The turbulent transport is inwards for both main ions and impurities, but the impurity ion inward transport is much weaker than the main ion inward transport. The neoclassical impurity transport for low charge number (Z) is outwards because of temperature screening, but inwards if the impurities are in the collisional regime (high Z). The total impurity transport, determined by a balance between turbulent and neoclassical transport, depends sensitively on the charge number of the impurity and the ratio of the ion density and temperature scale lengths, η_i.

Introduction

The presence of impurities in the edge region of tokamaks can be beneficial because a strongly radiating boundary distributes plasma power loss. But many tokamak discharges suffer from unwanted and uncontrollable impurity accumulation in the plasma core and this may lead to core radiation, flat radial distribution of temperature, fuel dilution and sometimes even disruptions. Impurity transport is critical for ITER and the issue of what governs the impurity transport should be given careful consideration.

Neoclassical transport is driven by parallel friction dynamics, and is not affected significantly by the fact that the ion cross-field transport is dominated by fluctuations. Thus it is clear that neoclassical and anomalous transport co-exist. The assumption that the total impurity transport is a linear sum of turbulence-driven transport and neoclassical transport has been confirmed experimentally. Reference [1] describes low-Z impurity transport in DIII-D, and shows that both types of transport have to be included to explain the observed transport phenomena.

Turbulent transport is usually much stronger than what neoclassical theory predicts. However, it has been found in many tokamak experiments [2, 3, 4] that in advanced scenarios impurity fluxes in the core may be of the order of the predictions of neoclassical theory. Thus, there is a strong motivation to compare neoclassical and turbulent impurity fluxes to determine which mechanism is stronger in ITER-like experimental situations.

In this work we compute the impurity transport from neoclassical theory and compare it with transport calculated from the reactive drift wave model of turbulent transport for a specific ITER-like scenario. As we will show, the total (neoclassical+turbulent) impurity flux depends sensitively on the charge number of the impurity and the ratio of the ion density and temperature scale lengths, η_i.

Neoclassical transport

Neoclassical ion transport is dominated by collisions with impurities since ion-impurity collisions are more frequent than ion-electron collisions. From the ambipolarity condition it follows that the impurity flux is oppositely directed to the ion flux $\Gamma_i = -Z\Gamma_z$. In the absence of the thermal force this should lead to impurity accumulation ($n_z \sim n_i^Z$, where n_z and n_i are the impurity and background ion densities). The accumulation can be reduced or avoided if the coefficient in front of the thermal force is negative. The outward flow induced by the thermal force, referred to as temperature screening, normally requires that the ions are collisionless and its effectiveness depends on the impurity charge and the fraction of impurities in the plasma.

Impurity-impurity collisions are more frequent than ion-ion collisions, so that heavy impurities are usually more collisional than the ions: if $T_z \simeq T_i$, $\nu_\star^z = \nu_\star^i Z^{3/2}(1+\alpha\sqrt{Z})$, with $\alpha = n_z Z^2/n_i$. The normalized collisionality is defined as $\nu_\star^a = \nu_a qR/v_{Ta}\epsilon^{3/2}$, where $\nu_a = \sum_b \nu_{ab}$ is the collision frequency, $\nu_{ab} = n_b e_a^2 e_b^2 \ln\Lambda/(4\pi\epsilon_0^2 m_a^2 v_{T>} v_{Ta}^2)$, where $v_{T>}$ denotes the larger of the thermal velocities v_{Ta} and v_{Tb}, $\ln\Lambda$ is the Coulomb logarithm, q is the safety factor, R is the major radius and $\epsilon = r/R$ is the inverse aspect ratio. In today's tokamak experiments, impurities tend to lie in the collisional regime ($\nu_\star^z\epsilon^{3/2} \gg 1$). However, for ITER-like parameters (density $n_i = 10^{20}$ m^{-3}, temperature $T_i = 10$ keV, $q = 2$, $R_0 = 6$ m, $\alpha \simeq 0.7$ and $\epsilon^{3/2} \simeq 0.3$), low-$Z$ impurities are collisionless ($\nu_\star^z < 1$) up to charge number $Z = 11$.

In this work we calculate the impurity transport in a plasma containing background ions (i) and electrons (e) and one species of impurity (z). The ion particle flux $\mathbf{\Gamma}_i = n_i \boldsymbol{V}_i$ is given by [5], $\langle \mathbf{\Gamma}_i \cdot \nabla\psi\rangle = \sum_{a=i,z;k=1,2} L_{1k}^{ia} A_k^a$, where $A_1^a = \partial \ln p_a/\partial\psi$ and $A_2^a = \partial \ln T_a/\partial\psi$ are the thermodynamic forces, n_a, p_a and T_a are density, pressure and temperature, $\psi = -RA_\varphi$ is the poloidal flux-function, $\boldsymbol{B} = I\nabla\varphi + \nabla\varphi\times\nabla\psi$ is the magnetic field, $L_{jk}^{ab} = 3\langle(\nabla_\parallel B)^2\rangle(I^2 T_b/e_a e_b B_0^4)\left(\mu_{aj}\mu_{bk}/\mu_1 - \mu_{a,j+k-1}\delta_{ab}\right)$, is the transport matrix, $\mu_1 = \mu_{i1} + \mu_{z1}$, $B_0 = \langle B^2\rangle^{1/2}$ and $\langle\ldots\rangle$ is the flux-surface average.

Banana regime

The neoclassical viscosity coefficients in the banana regime are

$$\mu_{ak} = \frac{m_a n_a B_0^2}{3\langle(\nabla_\parallel B)^2\rangle}\frac{f_t}{f_c}\left\{\nu_D^a\left(x_a^2 - \frac{5}{2}\right)^{k-1}\right\}, \tag{1}$$

$\nu_D^a = \sum_b \nu_D^{ab}$ and $\nu_D^{ab}(v) = \hat{\nu}_{ab}[\phi(x_b) - G(x_b)]/x_a^3$ is the deflection frequency, with $\phi(x)$ and $G(x)$, the error and Chandrasekhar functions, $x_a = v/v_{Ta}$ the normalized velocity, $\hat{\nu}_{ab} = \nu_{ab} v_{T>}/v_{Ta}$, $f_c = \frac{3}{4}\int_0^{\lambda_c}\lambda d\lambda/\langle\sqrt{1 - B\lambda/B_0}\rangle$, is the effective fraction of the circulating particles, $f_t = 1 - f_c$ and $\lambda_c = B_0/B_{\max}$. The braces denote the velocity integration operator $\{F(v)\} = \frac{8}{3\sqrt{\pi}}\int_0^\infty F(xv_{Ta})e^{-x^2}x^4dx$. The impurity flux is given by

$$\langle \mathbf{\Gamma}_z \cdot \nabla\psi\rangle = \frac{f_t}{f_c}\frac{n_iT_iI^2\xi_z\left\{\tilde{\mu}_{z1}[\tilde{\mu}_{i1}(\ln p_i)' + \tilde{\mu}_{i2}(\ln T_i)'] - \frac{T_z\tilde{\mu}_{i1}}{T_iZ}[\tilde{\mu}_{z1}(\ln p_z)' + \tilde{\mu}_{z2}(\ln T_z)']\right\}}{m_iZ\Omega_i^2\tau_{ii}(\tilde{\mu}_{i1}+\xi_z\tilde{\mu}_{z1})}, \quad (2)$$

where prime denotes derivative with respect to ψ, $\tilde{\mu}_{aj} = 3\langle(\nabla_\parallel B)^2\rangle\tau_{aa}f_c(f_tm_an_aB_0^2)^{-1}\mu_{aj}$, $\tau_{aa} = 3\sqrt{\pi}/4\hat{\nu}_{aa}$, $\xi_z = \tau_{ii}m_zn_z(\tau_{zz}m_in_i)^{-1}$ and $\Omega_i = eB_0/m_i$. The normalized viscosity coefficients are $\tilde{\mu}_{ij} = m_j^{ii} + m_j^{iz}\alpha$ and $\tilde{\mu}_{zj} = (m_j^{zi}/\alpha\sqrt{Z}) + m_j^{zz}$, with

$$m_1^{ab} = \sqrt{1+x_{ab}^2} + x_{ab}^2\ln\left[x_{ab}/\left(1+\sqrt{1+x_{ab}^2}\right)\right], \quad m_2^{ab} = 1/\sqrt{1+x_{ab}^2} - \frac{5}{2}m_1^{ab}, \quad (3)$$

where $x_{ab} = v_{Tb}/v_{Ta}$. The term proportional to the ion temperature gradient in Eq. (2) leads to outward transport of impurities (temperature screening). The inward flux driven by the impurity temperature gradient can be neglected, since

$$Z\frac{1+\tilde{\mu}_{i2}/\tilde{\mu}_{i1}}{1+\tilde{\mu}_{z2}/\tilde{\mu}_{z1}}\frac{T_i'}{T_z'} \simeq 2ZT_i'/T_z' \gg 1 \quad (4)$$

is satisfied in the parameter region of interest. Furthermore, if $|n_i'/n_i| \gg (T_i/ZT_z)|n_z'/n_z|$, also the flux driven by the impurity density gradient can be neglected. A criterion for the outward transport of impurities can then be derived to be $n_i'(\eta_i - \eta_i^t) < 0$, where $\eta_i = (n_iT_i'/n_i'T_i) = L_{ni}/L_{Ti}$ is the ratio between the ion density and temperature scale lengths and $\eta_i^t \equiv -\tilde{\mu}_{i1}/(\tilde{\mu}_{i1}+\tilde{\mu}_{i2})$.

If the impurity-ion density ratio n_z/n_i is constant, then $\xi_z = \alpha^2\sqrt{m_z/m_i}(T_i/T_z)^{3/2} \simeq \alpha^2\sqrt{Z}$ is strongly dependent on Z and the flux increases with Z. This behaviour has been confirmed experimentally [4]. However, if $Z_{\text{eff}} \equiv (n_zZ^2+n_i)/(n_zZ+n_i)$ is assumed to be constant, the fraction of impurities n_z/n_i decreases with increasing Z, and $\xi_z \simeq \sqrt{Z}$. As a consequence, the neoclassical transport decreases weakly with increasing Z.

Collisional regime

Even in ITER, impurities with high Z may be collisional, specially at the edge, where the temperature is low. In the collisional regime the viscosity coefficients are

$$\mu_{ak}^c = \frac{2p_a}{5}\left\{\frac{x_a^2}{\nu_T^a}\left(x_a^2 - \frac{5}{2}\right)^{k-1}\right\}, \quad (5)$$

where $\nu_T^a = \sum_b\left(2\nu_s^{ab} - \nu_\parallel^{ab} + \nu_D^{ab}\right)$, $\nu_s^{ab} = 2\hat{\nu}_{ab}(T_a/T_b)(1+m_b/m_a)G(x_b)/x_a$, and $\nu_\parallel^{ab} = 2\hat{\nu}_{ab}G(x_b)/x_a^3$. The impurity flux is given by

$$\langle \mathbf{\Gamma}_z^c \cdot \nabla\psi\rangle = \frac{3\langle(\nabla_\parallel B)^2\rangle T_iI^2p_z\tau_{zi}\left\{\tilde{\mu}_{z1}^c[\tilde{\mu}_{i1}^c(\ln p_i)' + \tilde{\mu}_{i2}^c(\ln T_i)'] - \frac{T_z\tilde{\mu}_{i1}^c}{T_iZ}[\tilde{\mu}_{z1}^c(\ln p_z)' + \tilde{\mu}_{z2}^c(\ln T_z)']\right\}}{Ze^2B_0^4(\tilde{\mu}_{i1}^c + p^*\tilde{\mu}_{z1}^c)}$$

where the normalized viscosity coefficients are defined as $\tilde{\mu}_{aj}^c = p_a\tau_{ai}\mu_{aj}^c$, $p^* = p_z\tau_{zi}/p_i\tau_{ii} \simeq \alpha/Z^{3.5}$. Since the viscosity coefficients are positive, and normally the temperature and density gradients are negative, the flux is inwards. Note, that the flux is proportional to the impurity density, and if Z_{eff} is constant, the flux is very rapidly decreasing with increasing Z.

Anomalous transport in the reactive drift wave model

The reactive model used here [6] (usually called Weiland model) has been used extensively in describing the present international tokamak database (JET, ASDEX, DIII-D) and for making ITER predictions [7]. It uses an "advanced" reactive fluid model where "advanced" here refers to the rule for closure which allows us to use the model close to the fluid resonance in the collisionless case. In the version used here it has two independent ion species with the same physics included for both. The particle transport for the main species was tested successfully on JET discharges in Ref. [8]. The particle pinch depends strongly on the magnetic drift frequency. Because of this, species with larger Z have a weaker particle pinch thus giving a favourable net effect on the effective Z. The particle pinch is particularly relevant for ITER since central fuelling will not be possible there. In fact the particle pinch has been found to improve ITER performance significantly.

The transport coefficients used in the calculations are derived using quasilinear theory [9, 10, 11]. The impurity diffusion coefficient D_z, defined by $\Gamma_z = -D_z \partial n_z/\partial r$ is given by

$$D_z = 2\bar{\gamma}^3 \frac{\rho_s c_s}{R k_y} (\Delta_1 - \Delta_T \eta_z + 2\Delta_2 L_{nz}/R), \tag{6}$$

where $\rho_s = c_s/\Omega_i$, c_s is the sound speed, γ and $\boldsymbol{k}$ are the linear growth rate and the wave-number of the unstable mode, x and y are slab coordinates corresponding to radial and poloidal coordinates, and the components of the wave-number are assumed to be $k_x\rho_s \simeq k_y\rho_s \simeq \sqrt{0.1}$, $L_{na} = -n_a/n_a'$ and $L_{Ta} = -T_a/T_a'$ are the density and temperature scale lengths for particle species a and $\eta_z = L_{nz}/L_{Tz}$, $\Delta_T = 2\tau_z\left(\bar{\omega}_r + 5\tau_z/3\right)/|\bar{N}_z|^2$, the overbar denotes normalization with respect to the electron magnetic drift frequency $\omega_{De} = 2k_yT_e/eBR$, $\tau_z = T_z/(ZT_e)$,

$$\Delta_1 = \left[\bar{\omega}_r^2 + \bar{\gamma}^2 + 14\bar{\omega}_r\tau_z/3 + 55\tau_z^2/9\right]/|\bar{N}_z|^2,$$

$$\Delta_2 = -\left[\bar{\omega}_r^2 + \bar{\gamma}^2 + 10\bar{\omega}_r\tau_z/3 + 35\tau_z^2/9\right]/|\bar{N}_z|^2,$$

where $|\bar{N}_z|^2 = N_{zr}^2 + N_{zi}^2$, with $N_{zr} = \bar{\omega}_r^2 - \bar{\gamma}^2 + 10\tau_z\bar{\omega}_r/3 + 5\tau_z^2/3$ and $N_{zi} = 2\bar{\gamma}\left(\bar{\omega}_r + 5\tau_z/3\right)$. These expressions are in agreement with the corresponding ones given in Ref. [11, 12].

The diffusion coefficient derived above is for the electrostatic case, but electromagnetic effects only influence the unstable wave frequency and electron diffusivity, and have no effect on the expression for the impurity diffusion coefficient. The frequency and growth rate of the unstable mode, $\bar{\omega} = \bar{\omega}_r + i\bar{\gamma}$, are determined numerically, including electromagnetic effects.

It is well known that the growth-rate of the main ion temperature gradient (ITG) mode is reduced by dilution [9]. This would tend to reduce the turbulent particle transport. However, for sufficiently large impurity density the impurity ITG takes over. The growth-rate of this mode increases with impurity density and accordingly also the turbulent particle transport increases. Thus, although the impurity density does not appear explicitly in our formulas, it is an important parameter. In the following section, the neoclassical transport will be compared with numerical calculations of the turbulent transport for ITER-like parameters and different impurity species. In these calculations we keep $Z_{\text{eff}} \simeq 1.7$ constant.

Impurity flux in ITER

For a specific high-Q ITER-like scenario [13], with minor radius $a = 2$ m, major radius $R = 6.2$ m, and magnetic field at the axis $B = 5.3$ T, the radial temperature and density profiles are given in Fig. 1. For the ITER scenario we selected, the density profile is slightly hollow and is much flatter than the temperature profile. For flat density profiles, η_i is large and the neoclassical transport in the banana regime (low-Z) is outwards. The reason for the outward flow is temperature screening, that is effective when $\eta_i > \eta_i^t \simeq 3.5$, if both the ion density and temperature gradients are negative. Note that even if the density gradient is locally positive $n_i'(\eta_i - \eta_i^t) < 0$ is satisfied, because η_i is then negative (assuming that the temperature gradient is still negative). However, it is interesting to note, that a more peaked density profile reduces the effect of temperature screening, and should reduce the outward transport. The transport due to the impurity gradients is more than an order of magnitude lower than the transport due to the ion gradients for this specific ITER-scenario.
The turbulent transport is caused by the ITG mode and trapped electron (TEM) mode. The growth rate of the ITG-mode is considerably larger than the growth rate of the TEM-modes and its real frequency is negative, while the real frequencies of the TEM-modes are positive. The impurity transport is inwards when $\Delta_1 - \Delta_T \eta_z + 2\Delta_2 L_{nz}/R < 0$, which is satisfied by impurities with any Z in this specific ITER-like scenario. Figure 1 shows the neoclassical and the numerically calculated turbulent impurity particle transport, as function of the normalized radius for impurity charges $Z = 6,\ 54$. It is interesting to note that for low-Z, neoclassical and turbulent transport have opposite signs. The numerical

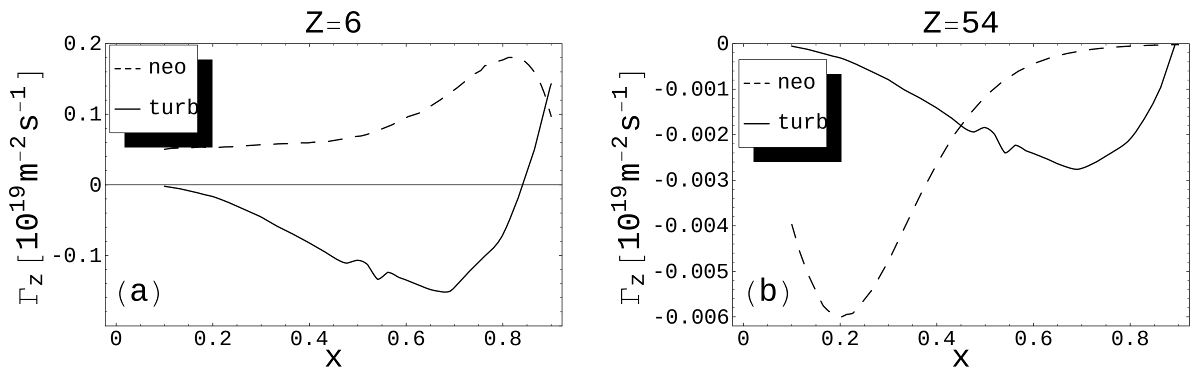

Figure 1: *Neoclassical (dashed) and turbulent (solid) impurity particle transport as function of normalized radius $x = r/a$.*

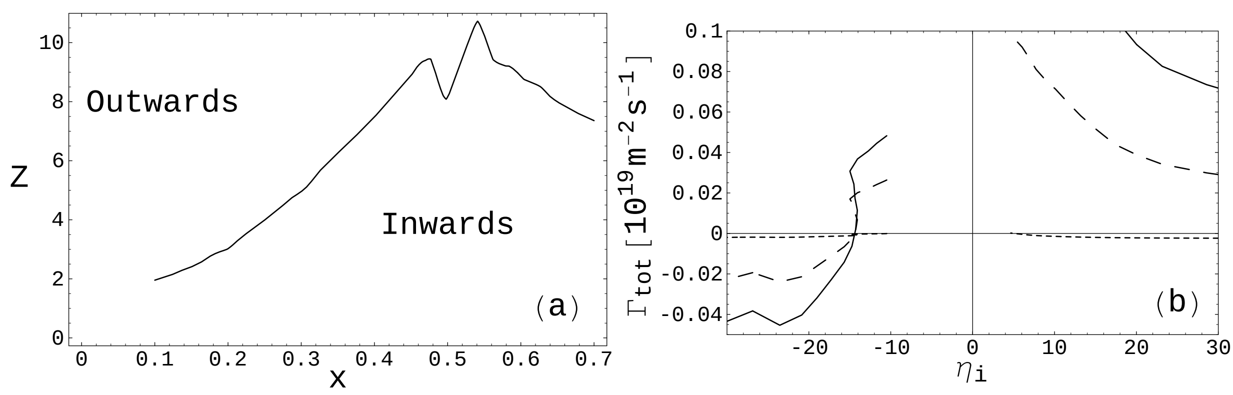

Figure 2: *(a) Impurity charge number for which the outward neoclassical transport dominates over the inward turbulent transport, as function of normalized radius $x = r/a$. (b) Total (turbulent+neoclassical) impurity transport as a function of η_i, for $Z = 6$ (solid), $Z = 10$ (dashed), $Z = 54$ (dotted). For large Z, the impurity transport is always inwards, but weak. For low Z, the impurity transport depends sensitively on η_i.*

calculations show, that turbulent transport is dominated by the unstable ITG-mode. The convective part of the transport, proportional to Δ_2 dominates, and that gives an inward flux of impurities. The terms proportional to Δ_1 and Δ_T give rise to outward transport (for the ITG-mode), but they are negligible inside the radius $r/a < 0.7$. Noting that for $r/a < 0.7$, $\Delta_2 \simeq -1/(\bar{\omega}_r^2 + \bar{\gamma}^2)$, we can rewrite the convective part of the flux as

$$\Gamma_z^{turb} \simeq -\frac{2\bar{\gamma}^3}{\bar{\omega}_r^2 + \bar{\gamma}^2} \frac{T_{\rm keV}^{3/2} n_z}{B^2}, \tag{7}$$

where $T_{\rm keV}$ is the ion temperature in keV. The flux given in Eq. (7) is approximately equal to the total turbulent flux inside the radius $r/a < 0.7$. Outside this radius, the terms proportional to Δ_1 and Δ_T become comparable to the convective part, and reduce the inward transport, so much that it sometimes even changes sign at the edge.

Assuming flat density profiles, so that the flux driven by the ion density gradient can be neglected, the neoclassical flux in the banana regime can be approximated as

$$\Gamma_z^{neo} \simeq -2 \cdot 10^{16} \frac{f_t}{f_c} \frac{q^2 n_{19}^2 T'_{\rm keV}}{Z B \epsilon^2 T_{\rm keV}^{3/2}} \tag{8}$$

for $r/a < 0.7$, where n_{19} is the ion density in units of 10^{19} m^{-3}. Using these approximate expressions for the neoclassical and turbulent transport we can determine the charge number for which the outward neoclassical transport is larger than the inward turbulent transport:

$$Z > Z_{\rm eff} + 10^3 \frac{Z_{\rm eff} - 1}{B} \frac{\epsilon^2}{q^2} \frac{f_c}{f_t} \frac{\bar{\gamma}^3}{\bar{\omega}_r^2 + \bar{\gamma}^2} \frac{T_{\rm keV}^3}{T'_{\rm keV} n_{19}} \tag{9}$$

Figure 2a shows Z as a function of normalized radius. For low Z impurities, the inward turbulent transport dominates. However, the main ion inward transport is at least an order of magnitude larger.

The growth rate of the unstable ITG-mode increases with η_i, so that the turbulent transport (which is normally inwards) increases. Even if η_i is large, leading to strong outward neoclassical transport, the resulting (turbulent+neoclassical) transport can be inwards, if the the turbulent transport is large enough to dominate over neoclassical transport. Figure 2b shows the total (turbulent+neoclassical) impurity transport as a function of η_i, for impurity charges $Z = 6,\ 10,\ 54$. For low Z, the impurity transport depends sensitively on η_i. The direction of the impurity flux is inwards if η_i is large and negative (flat and slighty hollow profiles), and the threshold is at $\eta_i \simeq -15$. Below $\eta_i \simeq -15$ turbulent transport dominates and the total impurity transport is inwards. For large and positive η_i (outside $r/a = 0.7$), inwards transport caused by the convective term Δ_2 is counteracted by the outwards transport caused by Δ_1 and Δ_T, and the neoclassical transport so that the total transport is outwards.

Our expression for the impurity diffusion coefficient shows that the magnitude (and sometimes even the direction) of the anomalous flux depends on the sign of the real frequency of the unstable mode, which is different for the ITG and TEM modes. The TEM-mode, with a positive real frequency, gives rise to an inward flux, while the ITG-mode can give rise to both inwards and outwards flux depending on the relative magnitude of the terms Δ_1, Δ_T and Δ_2. For the chosen ITER-profile the ITG-mode is dominant, and the anomalous flux is inwards, except for low-Z impurities in the edge plasma.

Conclusions

The direction of the total impurity transport depends on the impurity charge number Z and the ratio of ion density and temperature scale lengths η_i. If Z is high (collisional impurities), both turbulent and neoclassical transport are inwards for all η_i. If Z is low (collisionless impurities), the direction of the total impurity transport depends sensitively on η_i. If $\eta_i \gtrsim 3.5$, the direction of the total transport is outwards. If $0 < \eta_i \lesssim 3.5$, both neoclassical and turbulent impurity transport are inwards. If η_i is negative, the direction of the transport depends on the magnitude of η_i. If $|\eta_i| \lesssim 15$ the total transport is outwards, but if $|\eta_i| \gtrsim 15$ (for flat and hollow density profiles), turbulent transport dominates over neoclassical and the total transport is inwards.

In this work we have only determined the direction and magnitude of the impurity transport for a given ITER-scenario, at a specific time, and we did not analyze the evolution of the impurity profiles in time. If the density profile becomes more peaked as the turbulence drives the main ions inwards, η_i changes, and then both the direction and magnitude of the impurity transport will change.

Our analysis assumes that the effect of the interaction between different impurity species and charge states can be neglected. This assumption is justified when the impurity density is low, so that collisions among different species may be neglected. Furthermore, we neglect the effect of plasma rotation, since it is not expected to be very strong in ITER.

Our conclusions are in qualitative agreement with the conclusions of [14]. In Ref. [14]

impurity behaviour was numerically calculated for ITER operational scenarios and it was shown that for flat density profiles, temperature screening prohibits impurity accumulation in the core. However, our analysis shows, that depending on the sign and magnitude of η_i, even for for low Z, turbulent transport may dominate over neoclassical, and the direction of the impurity particle transport may be inwards. For collisional impurities (high-Z), both neoclassical and turbulent transport is inwards. However, the turbulent transport of main ions is usually also inwards and dominates the effect on the charge balance.

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