Pfirsch-Schlüter impurity transport in stellarator edge plasmas with large radial gradients

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Abstract. Large radial gradients of the bulk ion temperature and density in edge plasmas cause heavy impurity ions to redistribute themselves within flux surfaces, thereby making the impurity density vary poloidally (and, in a stellarator, toroidally). This redistribution reduces the radial impurity flux. In this paper, the effects of stellarator geometry on this mechanism are investigated, which lead to qualitatively different results compared with axisymmetric systems, in which the plasma can rotate freely. We derive analytic expressions for the radial impurity flux and the impurity density. The resulting differential equations are solved analytically in some limiting cases and numerically for W7-X and W7-AS.

1. Introduction
Toroidal edge plasmas are often characterised by large radial gradients of the bulk ion density and temperature. In fusion relevant experiments, these gradients can easily become larger than allowed for by conventional neoclassical theory based on a small-gyroradius expansion, \( \delta_a \equiv \rho_{a\theta}/L_\perp \ll 1 \), of the kinetic equation, where \( \rho_{a\theta} \) is the poloidal gyroradius and \( L_\perp \) the radial scale length of the density and temperature gradients. This problem may be of particular interest in the context of the H-mode. Although it is fundamentally difficult to construct a rigorous neoclassical transport theory if \( \delta_a \) is not a small parameter, it is possible to extend conventional theory to include cases of larger gradients. In this new ordering, \( \delta_i \) is still treated as small, though not as the smallest expansion parameter any more, as is implicitly assumed in conventional theory. Products of \( \delta_i \) with large parameters can easily be of order unity. In the present work, we take \( \Delta_i \equiv \delta_i \bar{\nu}_{ii}Z^2 = O(1) \), where \( \bar{\nu}_{ii} \equiv L_{ii}/\lambda_{ii} \) is the collisionality, which is large in the Pfirsch-Schlüter regime, \( \lambda_{ii} \) being the ion mean free path and \( L_{ii} \) the connection length, and \( Z \) is the impurity charge. The consequence is that the lowest order impurity distribution function is only locally Maxwellian, contrary to the conventional case where all lowest order quantities are flux functions. In practice, as a consequence of the large gradients, the impurities start developing density variations within the flux surface, which, depending on the plasma conditions, can lead to an accumulation of impurities at certain points on the flux surface. In tokamaks, this redistribution has previously been predicted to lead to impurity accumulation of the order of up to 30% of the total density at the high-field side of the torus [1, 2], a result which is in qualitative agreement with experimental results of present machines such as Alcator C-mod or MAST. However, there has been no work at all on how this effect is affected by stellarator geometry, and the calculations presented in this paper are aiming at calculating this effect. As a stellarator plasma, contrary to the tokamak case, cannot rotate freely [3] but instead has a
radial electric field which adjusts itself so as to make the radial transport ambipolar, the impurity redistribution is different in a stellarator due to effects from the radial electric field which cancel in axisymmetric systems. The remainder of this paper is organised as follows. In section 2, the kinetic theory is described and a differential equation for the impurity density variation is derived. This equation is solved, first in different analytical limits in section 3, and then fully with the help of numerical tools in section 4. The results are discussed and summarised in section 5.

2. Kinetic equations

We consider a stellarator plasma in the collisional regime consisting of hydrogenic bulk ions and a single species of heavy, highly charged impurities with charge $Z \gg 1$. The effect of electron collisions on the other species is small and therefore neglected, and the impurities are assumed to be not too numerous, so that the assumption $Z^2 n_e/n_i \ll 1$ holds (trace impurities). The drift kinetic equation for each species is

$$C_a(f_a) = v_{\parallel} \nabla \cdot f_a + v_d \cdot \nabla f_a - \frac{e_a}{m_a} \nabla \phi \frac{\partial f_a}{\partial v_{\parallel}},$$  

where $\phi$ is the electric potential, $e_a$ the charge of particle species $a$ and $v_d$ is given by

$$v_d = \frac{E \times B}{B^2} + \frac{v_{\perp}^2}{2 m_a} \frac{B \times \nabla B}{B^2} + \frac{v_{\parallel}^2}{\Omega_a} \frac{B \times \kappa}{B},$$

where $E$ and $B$ denote the electric and the magnetic field, respectively, $\Omega_a$ is the gyrofrequency and $\kappa \equiv (b \cdot \nabla) b$ is the magnetic curvature. $b$ is the unit vector along the magnetic field, $v_\parallel = b \cdot v$ and $\nabla_\parallel = b \cdot \nabla$. These equations are solved employing the ordering $\delta_i \ll 1$, $\Delta_i = O(1)$. For the bulk ions, this ordering corresponds to the conventional ordering, leading to a Maxwellian distribution in lowest order, and the first order equation

$$C_i(f_{i1}) = v_{\parallel} \nabla \cdot f_{i1} + v_d \cdot \nabla f_{i0} + \frac{e_i}{T_i} v_{\parallel} \nabla \cdot f_{i0}$$

has the solution [4]

$$f_{i1} = -\frac{2}{5} \frac{m_i}{p_i T_i} q_{i||} v_{||} f_{i0} \left( L_1^{(3/2)} \left( x_i^2 \right) - \frac{4}{15} L_2^{(3/2)} \left( x_i^2 \right) \right) + \left( \frac{p_i}{p_{i0}} + \frac{m_i}{T_i} v_i V_{i||} + \left( x_i^2 - \frac{5}{2} \right) \right) f_{i0},$$

where $L_j^{(k)}$ denote the Sonine polynomials (generalised Laguerre polynomials), $x \equiv v/v_{th}$, where $v_{th}$ denotes the thermal velocity. Since we consider trace impurities, ion-impurity collisions are negligible compared with ion self collisions, so that the solution corresponds to the pure-plasma solution. The parallel flow velocity $V_{i||}$ and the parallel heat flow $q_{i||}$ can be determined using particle conservation and the approximate conservation of energy in collisions between particles with disparate masses. It is convenient to use the equilibrium current $j_0$ and the equilibrium pressure $p_0$ to introduce a geometric quantity $u$, defined by

$$h \equiv \frac{j_0}{p_0} = \frac{1}{p_0} \left( \frac{b \times \nabla p_0}{B} + j_0 b \right) \equiv \frac{b \times \nabla \psi}{B} + uB,$$

where a prime denotes derivation with respect to the radial spatial coordinate $\psi$. Since the divergence of the equilibrium current must vanish, $\nabla \cdot h = 0$, $u$ must satisfy

$$\nabla_\parallel u = \frac{1}{p_0} \nabla_\parallel \left( \frac{j_0}{B} \right) = \frac{2}{B^2} (b \times \nabla \psi) \cdot \nabla \ln B.$$

(2)
In this notation, particle and energy conservation yield [5]
\[
B \nabla_{\parallel} \left( \frac{n_a V_{a1}}{B} - \frac{p_a}{e_a} A_{a1} u \right) = 0, \quad B \nabla_{\parallel} \left( \frac{q_{a2}}{B T_a} - \frac{5 p_a}{2 e_a} u A_{a2} \right) = 0,
\]
and thus for the parallel ion flow velocity and heat flux
\[
V_{i\parallel} = \frac{T_i}{e_i} A_{i1} u B + K_i(\psi) B,
\]
\[
\frac{q_{i\parallel}}{T_i} = \frac{5 P_i}{2 e_i} A_{i2} \left( u B - B \frac{\langle u B^2 \rangle}{\langle B^2 \rangle} \right),
\]
where the thermodynamic forces are defined as
\[
A_{a1} = \frac{d \ln p_a}{d \psi} + \frac{e_a}{T_a} \frac{d \phi}{d \psi}, \quad A_{a2} = \frac{d \ln T_a}{d \psi}.
\]

Since, for highly charged impurities, the ion and impurity temperatures are nearly equilibrated, \( A_{i2} \approx A_{a2} \). The integration constant in the equation for the heat flux was determined from the requirement that \( \langle B q_{i\parallel} \rangle = 0 \), where angular brackets denote an average over the flux surface, and, in the trace impurity limit, \( K_i(\psi) \) can, be determined from the next-order equations [4]
\[
K_i = -\frac{T_i n_i}{e_i} \left( A_{i1} + 1.82 A_{i2} \right) \frac{\langle u (\nabla_{\parallel} B)^2 + \frac{4}{5} \nabla_{\parallel} u \nabla_{\parallel} B^2 \rangle}{\langle (\nabla_{\parallel} B)^2 \rangle} - 0.05 A_{i2} \frac{\langle u (\nabla_{\parallel} B)^2 \rangle}{\langle (\nabla_{\parallel} B)^2 \rangle} - 1.77 A_{i2} \frac{\langle u B^2 \rangle}{\langle B^2 \rangle}.
\]

For the impurities, the lowest-order equation in the new ordering is
\[
C_z(f_z^{(0)}) = 0,
\]  
(3)

where \( C_z \) is the full linearised impurity collision operator. The solution to this equation is the \textit{perturbed} Maxwellian
\[
f_z^{(0)} = \left( \frac{p_z^{(0)}}{p_z} + \frac{m_z}{T_z} v_z V_z^{(1)} + \left( x_z^2 - \frac{5}{2} \right) \frac{T_z^{(1)}}{T_z} \right) f_z^{(0)},
\]  
(4)

leaving the lowest order density \( n_z^{(0)} \), temperature \( T_z^{(0)} \) and parallel flow velocity \( V_z^{(0)} \) free to vary on the flux surface as they are functions of the poloidal and toroidal angles, \( \theta \) and \( \psi \), respectively, as well as \( \psi \). Quantities ordered according to the new scheme are indicated by superscript indices whereas subscript indices symbolise the expansion in the conventional ordering \( \delta_i \ll 1, \Delta_i \ll 1 \). Quantities with a subscript 0 are always flux functions. Eq. (3) implies equal temperatures and flow velocities of all involved particle species, thereby making the lowest order impurity temperature a flux function, and the lowest order flow vanishes since this is true for the bulk ions. Therefore, the first quantity to vary on the flux surface when the gradients are large is the impurity density \( n_z \). The variation of the impurity temperature and flow velocity is one order smaller in \( \delta_i \) than the density variation.

Taking the particle moment of the impurity version of (1), one can exploit particle conservation to find
\[
\nabla \cdot \left( n_z^{(0)} \left( V_z^{(1)} b + \nabla_d \right) \right) = 0
\]
\[
\Rightarrow B \nabla_{\parallel} \left( \frac{n_z^{(0)} V_z^{(1)}}{B} \right) = -\frac{d \phi}{d \psi} \left( \frac{b \times \nabla \psi}{B} \cdot \nabla n_z^{(0)} - B n_z^{(0)} \nabla_{\parallel} u \right).
\]  
(5)
Both the impurity density and flow velocity are unknown, so another equation is needed, which can be obtained from the $\nu_\parallel$-moment of (1). It shows that the friction force is related to the impurity density variation via

$$
\int m_z v_\parallel C_{zi}(f_z^{(1)}) = R_{zi} = \int m_z v_\parallel^2 \nabla_\parallel f_z^{(0)} = \nabla_\parallel p_z^{(0)}
$$

$$
\Rightarrow \nabla_\parallel n_z^{(0)} = -\frac{1}{T_i} R_{zi}.
$$

Introducing the notation

$$
\tilde{v}(\psi) \equiv \frac{4}{3\sqrt{\pi}} \frac{m_i n_i}{e_i} \langle \tilde{v}_{iz} / n_z \rangle,
\quad \tilde{v}_{iz} \equiv \frac{n_z Z^2 e^4 \ln \Lambda}{4\pi \epsilon_0 m_i^2 v_{th,i}^3}
$$

$$
K_i^*(\psi) = K_i(\psi) + \frac{d\ln T_i}{d\psi} \langle u B^2 \rangle / \langle B^2 \rangle,
$$

$$
\gamma \equiv u + (A_{i1} - A_{i2})^{-1} K_i^*(\psi)
$$

and using a Lorentz operator plus a term guaranteeing momentum conservation to model ion-impurity collisions, one obtains from (5) and (6) the two equations

$$
\nabla_\parallel n_z = \tilde{v} \left((A_{i1} - A_{i2}) \gamma B n_z - n_z V_{z_\parallel} \right)
$$

and

$$
B \nabla_\parallel \left( \frac{n_z V_{z_\parallel}}{B} \right) = -\frac{d\phi}{d\psi} \left( \frac{b \times \nabla \psi}{B} \cdot \nabla n_z - B n_z \nabla_\parallel \gamma \right).
$$

In order to know the impurity density variation, eqs. (7) and (8) have to be solved. However, it is not possible to do so analytically for stellarator geometry. Therefore, different limits are solved analytically in the next section, and numerical results for the full equation will be given in section 4.

3. Analytical limits

It is possible to gain some useful information about how the impurity redistribution is affected by the various terms by considering different limits, i.e. strong or weak radial gradients or radial electric field, which will be done in the subsequent subsections.

3.1. Weak radial gradients

In the case of weak radial gradients, i.e. $\Delta_i \ll 1$, eq. (8) yields

$$
B \nabla_\parallel \left( \frac{n_z V_{z_\parallel}}{B} \right) \ll \frac{n_z V_{z_\parallel}}{L_\parallel},
$$

which leads to

$$
V_{z_\parallel} \approx \frac{B}{n_z} K_z(\psi).
$$

The constant $K_z(\psi)$ can be determined from the constraint that $\langle B \nabla_\parallel n_z \rangle$ must vanish, and becomes $K_z(\psi) = (A_{i1} - A_{i2}) \langle \gamma B^2 n_z \rangle / \langle B^2 \rangle$. The right-hand side of the remaining equation for $n_z$,

$$
\nabla_\parallel n_z = \tilde{v}(A_{i1} - A_{i2}) \left( \gamma n_z B - B \frac{\langle \gamma B^2 n_z \rangle}{\langle B^2 \rangle} \right),
$$
is small as well, and thus
\[ \nabla \parallel n_z \ll \frac{n_z}{L_i} \]
with the solution \[ n_z \approx n_z(\psi) \]. Thus, the conventional limit of weak gradients, leading to the densities being constant on flux surfaces, is correctly reproduced.

3.2. Large radial gradients, vanishing radial electric field
An interesting and analytically tractable limit is the case of small radial electric field, \( e_i/T_i d\psi/d\psi \ll d\ln n_i/d\psi \), in which the terms containing the perpendicular derivative in eq. (8) become negligible and the partial differential equations reduce to ordinary ones. Although this case would not occur in a realistic experimental equilibrium where density gradient and radial electric potential tend to cancel each other (ion root operation) and are thus of comparable magnitude, it is nonetheless enlightening to study this case as it has the appealing property of mathematically resembling the tokamak case and giving some fundamental insight into the different mechanisms involved in the redistribution process. In this limit, the right-hand side of (8) is approximately equal to zero, and thus the impurity flow velocity can be calculated in terms of the impurity density, leading to eq. (9) as in the opposite limit. The solution to this equation depends fundamentally on the properties of the function \( \gamma \), especially on whether \( \gamma \) has any zeroes. If this is not the case, and if the gradients are steep in the sense that \( \Delta_i \gg 1 \), the left-hand side of (9) is negligible due to the large multiplier \( A_{i1} - A_{i2} \) on the right-hand side. The solution then becomes rather simple,
\[ n_z \approx \langle \frac{1}{\gamma} \rangle^{-1} \frac{1}{\gamma}. \]
Employing the value for \( \gamma \) in the axisymmetric limit,
\[ \gamma|_{axisym} = -\frac{I(\psi)}{B^2(1 + 2.77d\ln T_i/d\psi)} \]
where \( I(\psi) \) is the toroidal current, reproduces the tokamak result found in [1] correctly.

However, if \( \gamma \) does have zeros, the problem is fundamentally different. As there are points at which the right-hand side of (9) vanishes, it is not possible to neglect the parallel gradient in these regions, in which a boundary layer forms. The calculation for this case, based on the method of integrating factors and an expansion around the points where \( \gamma \) vanishes, is given in the following. The result is that, in the limit of very large gradients, the impurities become strongly localised around these zeros, an effect which can be understood physically by noticing that the friction force, which is the drive for the redistribution, is proportional to \( \gamma \) and thus vanishes at these points. Due to periodicity, there must exist points from where all impurity ions are carried away, but also points at which they accumulate. In the limit \( \Delta_i \to \infty \), the impurity density becomes a delta distribution at the accumulation points.

This situation can in principle also occur in a tokamak, but parametric dependencies of \( \gamma|_{axisym} \) show that this is only possible if the radial temperature and density gradients have opposite signs, which is usually not the case.

4. Numerical solution of the full problem
To study realistic scenarios, in which the pressure gradient and the radial electric field are of comparable magnitude and approximately cancel each other, one has to resort to numerical means. This has been done via a Fourier decomposition with respect to the poloidal and toroidal
angle using the MConf library, which has been developed for transport analyses in stellarators [6]. The Fourier series was truncated after 54 components in both angles, and periodicity was used for the toroidal direction.

Fig. 1 shows the results for W7-AS for different values of $\tilde{v}(A_{i1} - A_{i2})a^2$. The plasma parameters were chosen to match experimental values in W7-AS during H-mode operation (ion root operation). For a bulk ion density of $5 \cdot 10^{19} - 1 \cdot 10^{20}$, a bulk ion temperature of $100eV$ and a radial density scale length of $2cm$ in the pedestal, realistic values for $\tilde{v}(A_{i1} - A_{i2})a^2$ lie between 0.01, corresponding to weak gradients, and 10 for very large gradients and high impurity charge. As an upper limit and to show what happens qualitatively in the limit of very large gradients and very high impurity charge, values of up to 100 have been included in the calculations. The flux surface was chosen to be $s = 0.9$, where $s$ is the magnetic flux normalised to the flux at the separatrix.

As is visible from the figure, for weak radial gradients the impurity density is nearly constant on the flux surface, and thus the limit of conventional theory is correctly recovered. A slight in-out asymmetry exists, with the impurities accumulating at the inboard side of the torus, but the overall density variation is moderate with only 5% variation. When the gradients get larger, the impurities accumulate at a certain toroidal angle. In the limit of very large gradients, the distribution function approaches a delta distribution at these points. When looking at the pattern of the function $\gamma$ for these plasma parameters, one finds that $\gamma$ crosses zero, and thus points of vanishing friction force exist, which explains the very strong accumulation of the impurities. In fig. 3, the corresponding radial impurity flux is plotted as a function of the largeness of the gradients. One can show that, in leading order, the particle flux across the field is given by [5]

$$\langle \Gamma_z \cdot \nabla \psi \rangle = \frac{1}{c_z} \langle uB_{zz} \rangle,$$

and this is still true even when the impurity density is no longer a flux function. In comparison with a conventional calculation, where the flux increases linearly with increasing gradients, it is reduced by the redistribution. However, even for extreme values of $\tilde{v}(A_{i1} - A_{i2})a^2$, the flux is still a monotonically increasing function of the gradients.

Qualitatively different results are obtained for W7-X. Since the order of magnitude of the radial gradients in this device can be expected to be comparable to that found in W7-AS, the same range of simulation parameters should be appropriate. In this parameter regime, one finds that $\gamma$ does not have any zeros. The impurity accumulation is thus not as strong as in W7-AS, leading to up to 15% density variation as shown in fig. 2, again for different radial gradients. The pattern of the redistribution has two regions of accumulation separated by elongated regions with reduced density. The corresponding impurity flux is shown in fig. 3. Interestingly, although the density variation is much smaller than in W7-AS, the effect on the radial transport is much more pronounced, leading to a considerable reduction of the impurity flux and thus making it a non-monotonic function of the radial gradients.

Running the code for tokamak devices leads to the results found previously of impurity density peaking on the high-field side of the torus [1], with an overall variation between 10–30%, depending mainly on the aspect ratio of the device.

From both simulations and the analytic formulas, it is obvious that the drive of the redistribution is parallel friction between the bulk ions and the impurities, as in a tokamak. However, the way in which the impurities are redistributed is qualitatively influenced by, on the one hand, the radial ion temperature gradient, and, on the other hand, the radial electric field, which does not play a role in axisymmetric configurations. The effect of the radial temperature gradient comes from its entering the constant $K_i^* (\psi)$. Thereby, it influences the magnitude and possibly even the sign of the friction force, which has a large impact on the redistribution if
\( \gamma \) is modified from being entirely positive (negative) to a state where both signs occur. The radial electric field influences the redistribution in two different ways. Since it also enters the constant \( K_i^*(\psi) \), it can directly affect the friction force in this way. Additionally, it drives an \( \mathbf{E} \times \mathbf{B} \) rotation, which varies on the flux surface and thereby changes the pattern of the redistribution. Therefore, the dependence of the impurity density on the radial electric field is rather complicated and analytically not tractable.

However, the numerical results suggest that, even when a radial electric field is included, the impurity redistribution and consequently also the radial particle transport are strongly affected by whether or not \( \gamma \), which is proportional to the friction force, has zeros. If this in not the case,
the density variations are moderate. The exact redistribution pattern depends on the magnetic geometry of the device. Regarding the radial impurity transport, as long as the gradients are weak, the relation between the gradients and the radial impurity flux is approximately linear. When the gradients get larger, the impurities are redistributed in such a way that they experience less friction. Therefore, the radial flux is reduced and becomes very small for large gradients. Mathematically, this is manifested by the fact that the left-hand side of (7), which is proportional to the friction force and thus to the particle flux, becomes negligible when the gradients are large enough.

If $\gamma$ has zeros, the friction force vanishes at certain points and drives the impurity distribution function towards a delta distribution at “half” the zeros, namely, at those toward which the friction force is directed. If the radial electric field is strong, this process can be counteracted by the $\mathbf{E} \times \mathbf{B}$ rotation, which carries the impurities away from these points. However, in the simulation for W7-AS, the ambipolar electric field seems to be unable to prevent strong accumulation. Although the redistribution slightly reduces the friction force, since the impurity flux now increases less rapidly than linear with increasing magnitude of the radial gradients, it is still a monotonic function. Unlike the case when $\gamma$ does not have any zeros, there exist regions where the left-hand side of (7) is not negligible (namely, where $\gamma$ vanishes). Thus, the radial flux cannot become as small as when $\gamma$ does not have any zeros. Again, whether or not this is the case depends on the magnetic geometry.

5. Conclusions & Summary

The presence of large gradients in the plasma edge region has a significant effect on heavy impurity ions. Their density develops variations within the flux surface of the order of up to $10 - 100\%$, depending on the device. The effect is qualitatively different from that previously found in tokamaks since the radial electric field plays a major role in the redistribution process, on the one hand by driving a non-constant (on the flux surface) $\mathbf{E} \times \mathbf{B}$ flow, which may carry particles away from regions of accumulation, and on the other hand by influencing the magnitude and especially the sign of the friction force, which is the main driving mechanism of the redistribution. The exact pattern of the impurity density on the flux surface depends sensitively on the exact geometry of the device. A crucial aspect for the redistribution process is whether there exist points at which the friction force vanishes. If this is the case, the redistribution can become much more strongly pronounced than otherwise. The radial impurity transport is greatly affected by the redistribution. Whereas it becomes very small when the gradients are large if there are no such points, it might still be a monotonically increasing function of the radial gradients when such points do exist, as in W7-AS, although the flux is still reduced in comparison with a situation without impurity redistribution. Apart from the effects due to the radial electric field, the main difference between tokamaks and stellarators with respect to impurity redistribution is the occurrence of strong localisation and the corresponding consequences for the transport for realistic values of the plasma parameters in stellarators. In tokamaks, this is in principle also possible, but only if the radial density and temperature gradients have opposite signs. The numerical solution of the full impurity density differential equation reproduces the analytical limits found correctly.

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