1. Introduction

When a plasma is confined by means of a magnetic field, \( B \), an electric field, \( \mathbf{E} = -\nabla \Phi \), invariably also arises. Because of the high conductivity of the plasma along the magnetic field, the electric field is mostly perpendicular to \( B \), but also has a small component within the flux surface. In other words, the electrostatic potential can be written as \( \Phi = \Phi_0(r) + \Phi_1 \), where \( \Phi_0(r) \) is constant on magnetic surfaces (labelled by the coordinate \( r \)) and \( \Phi_1 \) varies over such surfaces. This is true both in axisymmetric and non-axisymmetric magnetic fields, but the mechanisms creating the electric field are very different.
1. Radial electric field

We shall refer to the electric field perpendicular to the flux surface as radial, \( \mathbf{E}_0 = -\nabla \Phi_0 = E_r \nabla r \), and first note that, in an axisymmetric magnetic field such as that of a tokamak, plasma transport is independent of \( E_r \) to a good approximation. Both the collisional transport and that arising from gyrokinetic turbulence are independent of the radial electric field to lowest order in the normalised gyroradius, \( \rho_i = \rho_0/L \), and the Mach number \( M = V/V_{\text{Ti}} \), which we take to be much smaller than unity [3, 4]. Here, \( \rho_i \) denotes the ion gyroradius, \( V_{\text{Ti}} = \sqrt{T_i/m_i} \), the ion thermal velocity, \( \Omega_i \) the gyro-frequency, \( \Gamma \) the macroscopic length scale (such as the minor radius) and \( V \) the plasma flow velocity, the perpendicular component of which for the bulk ions with mass \( m_i \), density \( n_i \), temperature \( T_i \) and pressure \( p_i \) is equal to

\[
V_\perp = \frac{\mathbf{E} \times \mathbf{B}}{B^2}
\]

and is thus controlled by the radial electric field if this is large enough. If \( \mathbf{B} \) is axisymmetric, then the effect of \( E_r \) on the transport is first order in the small parameters \( \rho_i \) and \( M \). This property is usually referred to as intrinsic (or automatic) ambipolarity. There is a simple reason for it: in a coordinate system rotating toroidally with a velocity \( \mathbf{U} \), the electric field is equal to \( \mathbf{E} + \mathbf{U} \times \mathbf{B} \) (where \( \mathbf{E} \) denotes the field in the laboratory frame) and its radial component can be made to vanish by choosing \( \mathbf{U} \) appropriately. In such a frame, the physics is the same as in the laboratory frame, except that there is a centrifugal force and a Coriolis force. The former is quadratic in the Mach number and therefore does not matter to first order in \( M \), and the Coriolis force on a mass \( m \) moving with velocity \( \mathbf{v} \) is equal to

\[
\mathbf{F}_c = 2m\mathbf{v} \times \omega,
\]

where \( \omega \) is the angular rotation frequency corresponding to the velocity \( \mathbf{U} \). Because it has the same form as the Lorentz force on a charge \( q \), it can be accounted for in the kinetic equation by adjusting the magnetic field according to

\[
\mathbf{B} \rightarrow \mathbf{B} + \frac{2m}{q} \omega,
\]

which is a very small change, \( m\omega/qB \sim \rho_i M \). The effects of both the centrifugal and Coriolis forces are thus quadratic in the small parameters \( \rho_i \) and \( M \). The kinetic equation for the plasma in the rotating frame is thus locally identical to that in the laboratory frame to first order in these parameters, and we conclude that the radial electric field cannot affect the behaviour of the plasma in this order, at least not locally. (A sheared electric field can however have an effect on turbulence, and even an unsheared field can affect ITG stability through non-local effects [5].)

In a non-axisymmetric magnetic field, the neoclassical transport is not ambipolar unless the field is quasi-symmetric, and the radial electric field is set by the requirement that the ion and electron particle fluxes across magnetic surfaces should be equal. However, the turbulent transport remains ambipolar even in non-axisymmetric fields if the turbulent fluctuations satisfy the gyrokinetic equations [4, 6]. The radial electric field is determined by neoclassical transport processes alone in non-axisymmetric and non-quasisymmetric magnetic fields [7] (an exception occurs on small radial scales comparable to the ion gyroradius, on which zonal flows may arise). This is in stark contrast to tokamaks, where the radial electric field is controlled by the transport of angular momentum, which is a higher-order process in \( \rho_i \) and therefore difficult to calculate, both in neoclassical and in gyrokinetic theory [8, 9].

In a stellarator, the radial electric field affects the neoclassical particle flux of each species \( a \), which is governed by a transport law of the form

\[
\langle \mathbf{T}_a \cdot \nabla r \rangle = -n_a \sum_b \left[ D_{ab}^\text{ne} \left( \frac{d \ln n_b}{dr} - \frac{q_b E_r}{T_b} \right) + D_{ab}^\text{ke} \frac{d \ln T_b}{dr} \right],
\]

where \( n_a \) denotes the density, \( T_a \) the temperature, \( q_a = Z_a e \) the charge, and the sum is taken over all the species \( b \) present in the plasma. The terms with \( b \neq a \) are due to the friction along \( \mathbf{B} \) between the different species and are in stellarators usually negligible in comparison with the \( b = a \) term at low collisionality. The terms with \( b \neq a \) are therefore usually neglected in numerical codes [10]. The term proportional to the radial electric field is absent in axisymmetric systems but tends to cause relatively strong inward transport of highly charged impurities in stellarators, since \( E_r \) is usually negative.

1.2. Electric field within flux surfaces

The electric field within the magnetic surface, \( \mathbf{E}_i = -\nabla \Phi_i \), has received less attention in the literature. It is usually relatively small, but can have a substantial effect on highly charged impurities with charge numbers \( Z \gg 1 \). There are a few different mechanisms that can cause such a field to appear.

First, axisymmetric plasmas can rotate rapidly in the toroidal direction. In tokamaks with strong neutral-beam injection, the Mach number can become order unity, so that the centrifugal force becomes comparable to the pressure gradient. The bulk ions are then driven to the outboard side of each flux surface, and a poloidal electric field (directed toward the inboard side) arises to maintain quasi-neutrality [11, 12]. For heavy impurities, the force from this electric field is smaller than the centrifugal force, so the impurities are pushed to the outboard side of the flux surface.

Second, fast ions from neutral-beam injection or ion-cyclotron-resonance-heating (ICRH) usually have anisotropic pressure and are therefore not evenly distributed over flux surfaces. For instance, ICRH-heated minority ions reside mostly on the outboard side, and a poloidal electric field directed to the inboard side is again required to make the plasma quasi-neutral. Impurity ions therefore accumulate on the inboard side [13].

Third, even without fast rotation or fast ions, the plasma has a natural tendency to produce a poloidal electric field. In a tokamak, this electric field is relatively small, as can be seen from the \( \rho_i \)-expansion of the drift kinetic equation, which we write as
\[ \mathbf{R} \cdot \nabla f_a + \frac{v_1}{m_a} \frac{\partial f_a}{\partial v_1} = C_a(f_a), \]

where the derivatives are taken at constant magnetic moment, \( \mu = m_a v_1^2 / 2B \), and \( \mathbf{R} \) denotes the guiding centre position. To zeroth order in \( \rho_s \), there is no magnetic drift and the \( \mathbf{E} \times \mathbf{B} \) drift can be transformed away as described above, so that

\[ \mathbf{R} = v_1 \mathbf{b}, \]

\[ v_1 = -\frac{\mu}{m_a} \mathbf{b} \cdot \nabla B - \frac{Z_a e}{m_a} \mathbf{b} \cdot \nabla \Phi, \]

where \( \mathbf{b} = \mathbf{B} / B \), \( m_a \) denotes the mass. The electrostatic potential is determined by the quasineutrality condition

\[ \sum_a Z_a e f_a d^3 v = 0, \]

and one finds that \( \Phi_1 \) vanishes in this order [3], implying that \( e\Phi_1 / T \sim \rho_s \), where \( T \) is the temperature. From the first-order kinetic equation, one finds that the electrostatic potential is first order in the collisionality too, so that \( e\Phi_1 / T \sim \rho_s \nu_c \), where \( \nu_c = eL n_f T \) denotes the collisionality and \( \nu_f \) the thermal speed [14].

In a stellarator, the situation is more complicated, and the poloidally (and toroidally) varying part of the electrostatic potential can be significantly larger. This has to do with the mechanism through which the radial electric field causes the cross-field transport to be ambipolar.

The diffusion coefficients in equation (1) tend to be larger for the ions than for the electrons, which drives an inward-pointing radial electric field, which in turn reduces the flux of the ions and enhances that of the electrons. Eventually the radial electric field becomes large enough to establish ambipolar fluxes and the potential ceases to grow. It is clear from equation (1) that the required electrostatic potential must be of order

\[ \frac{e\Phi_0}{T} \sim 1. \]

On the level of particle trajectories, the reduction of the ion transport occurs because \( \mathbf{E}_0 \times \mathbf{B} \) drift convects locally trapped ions poloidally around the torus, and thereby limits the radial step size in their collisional random walk. However, as explained in [15, 16], the radial width of the resulting trajectories is such that the density develops an in–out asymmetry on each flux surface, and to keep the plasma quasineutral, a poloidal electric field is established. In these references, the electric field was calculated in the case of circular flux surfaces and was found not to scale with \( \rho_s \), but roughly as

\[ \frac{e\Phi_1}{T} \sim \frac{f_f \Delta B}{B}, \]

where \( \Delta B \) is the variation of the magnetic field strength over the flux surface and \( f_f \) the fraction of trapped particles. This ratio is usually smaller than unity by some considerable (but not very large) margin, so that the variation of the electrostatic potential over flux surfaces is modest. This variation causes an additional \( \mathbf{E}_d \times \mathbf{B} \) drift across the flux surfaces which adds to the radial neoclassical transport, but the effect is not very large for the bulk ions and electrons [16]. For moderate to highly charged impurity ions, the effect can however be substantial.

### 1.3. Effect on impurity ions

The neoclassical transport of impurity ions has long been an issue of concern. Since the total transport must be ambipolar, the outward flux of bulk ions must necessarily either be accompanied by a similar electron flux or be balanced by an inward impurity flux. In tokamaks, the neoclassical electron transport practically vanishes, and in stellarators, the inward electric field makes the second term in equation (1) for impurities a factor \( Z_a \) larger than the other terms, so in both cases impurity accumulation tends to arise. However, standard neo-classical theory assumes that all densities are constant over flux surfaces. Since the density tends to follow a Boltzmann distribution function within such surfaces,

\[ n_a \propto \exp \left( -\frac{Z_a e \Phi_1}{T_a} \right), \]

in particular impurities with \( Z_a \gg 1 \) will tend to develop impurity density variations in response to \( \Phi_1 \). Highly charged impurities also experience a relatively large parallel friction force from the bulk ions, which also leads to a density variation. Furthermore, the collisionless orbits also tend to get modified by \( \Phi_1 \), because the electric force along the field \( Z_a e \mathbf{b} \cdot \mathbf{E}_d \) can compete with the mirror force,

\[ \frac{Z_a e}{\mu} \nabla \Phi_1 \sim \frac{Z_a e \Phi_1}{T}, \]

if \( Z_a \Delta B / B \) is of order unity. Electrostatic trapping is then as important as magnetic trapping. For these reasons, the neo-classical transport of heavy impurity ions can be affected significantly, both in tokamaks [17–19] and in stellarators [20, 21]. In tokamaks, the most notable effects arise because of the potential variation caused by anisotropic fast ions, which can dramatically affect both the size and the magnitude of the transport [22].

### 2. Mathematical and numerical treatment

It is not entirely straightforward to construct an ordering of the various terms in the drift kinetic equation that is both rigorous and adequately describes the effect of the electric field whilst still retaining the radially local character of conventional neo-classical transport theory. Different alternatives were recently discussed and compared numerically by Landreman et al [23], who however neglected \( \Phi_1 \) in their treatment. We shall adopt their most complete model (called full trajectories in their paper), and extend it to include \( \Phi_d \). The full equations of guiding center motion are

\[ \mathbf{R} = v_1 \mathbf{b} + \frac{\mathbf{b} \times \nabla \Phi}{B} + \mathbf{v}_d \]

\[ \mathbf{v}_1 = -\frac{1}{m_a} \mathbf{R} \cdot (\mu v B + Z_a e \nabla \Phi), \]
\[ \dot{\mu} = 0, \]  
(6)

and the simplified local ones are

\[ R = v_1 b + \frac{b \times \nabla \Phi_0}{B}. \]  
(7)

\[ \dot{\nu}_1 = -\frac{\mu}{m_a}b \cdot \nabla B - \frac{v_1}{B^2}(b \times \nabla B) \cdot \nabla \Phi_0 - \frac{Ze_a}{m_a}b \cdot \nabla \Phi_1, \]  
(8)

\[ \dot{\mu} = 0. \]  
(9)

Equations (7)–(9) are obtained from (4)–(6) after suppressing the magnetic drift \( \nu_2 \) and the \( E \times B \) drift \( b \times \nabla \Phi_0/B \) in (4). This simplification assumes the smallness both of these terms and the perturbed portion of the distribution function in the drift kinetic equation, discussed below. Finally (8) comes from requiring phase-space volume conservation with the previous simplified guiding center, and implies neglecting the term \((v_1/B^2)(b \times \nabla B) \cdot \nabla \Phi_1\), embedded in (5).

### 2.1. The code EUTERPE and solution of the drift kinetic equation

For the integration of the equations of motion and calculation of the radial impurity fluxes and electrostatic potential variation \( \Phi_b \), the Monte Carlo \( \delta f \) particle-in-cell (PIC) code EUTERPE [24] has been employed. The details of the numerical method can be found in [25], but succinctly it can be summarised as follows.

The method considers a splitting of the distribution function \( f \) for any kinetic species present in the problem as \( f = f_0 + \delta f \), prescribing an analytically known part \( f_0 \) and a departure from this \( \delta f \), which is represented by a set of Monte-Carlo markers. The equation to solve for the \( \delta f \) part can be expressed in all generality as

\[ \frac{df}{dt} = -\frac{df_0}{dt} + C(f), \]  
(10)

with \( C(f) \) the collision operator.

The code is multi-species, the gyro-kinetic version is electromagnetic and considers the full flux surface and radial domain. The neoclassical version applied to the present problem is local instead, as no drift across the flux surface remains in equation (7), and binds the radial position of each marker to its value at the initialization. To solve equation (10) a standard two weight scheme [26, 27] is applied, with \( \delta f \) and \( f_0 \) represented by

\[ \delta f = \sum_p w_{1p} \delta(z - z_p)J^{-1}(z), \]  
(11)

\[ f_0 = \sum_p w_{2p} \delta(z - z_p)J^{-1}(z), \]  
(12)

with \( z = (R, v_1, \mu) \) the phase space coordinates, \( \delta \) the Dirac delta function, \( w_{1} \) and \( w_{2} \) the marker weights, \( p \) the marker index, \( J \) the phase space Jacobian. Denoting the set of phase space variables by \( z = (R, v_1, \mu) \), the full guiding centre equations (4) to (6) by \( z \) and the reduced local ones (7)–(9) by \( z_0 \), the following expressions for the evolution of the marker weights can be derived [25],

\[ \dot{w}_{1p} = -\frac{w_{2p}}{f_0} \frac{\partial f_0}{\partial \nu_0} \left( \frac{\partial \Phi_0}{\partial \nu_0} \right), \]  
(13)

\[ \dot{w}_{2p} = -\frac{w_{2p}}{f_0} \frac{\partial f_0}{\partial \nu_0} \left( \frac{\partial \Phi_0}{\partial \nu_0} \right), \]  
(14)

where the summation over repeated indices is assumed. In equations (13) and (14) the collision operator is assumed to consist only of the test particle term \( C(\delta f, f_0) \) describing the collisions of the \( \delta f \) on the \( f_0 \) background. This, in turn, has been approximated by a Lorentz pitch-angle scattering operator in the calculations below, where the collision frequency for the species \( a \) is the sum of the deflection collision frequencies with all plasma species \( b \) (including like-particle collisions for which \( a = b \)), that is \( \nu_{0a} = \sum_b \nu_{ab} \).

In a typical simulation the integration of the collisionless characteristics of each marker is then followed by a process simulating the pitch-angle scattering. This collisional step is carried out by assigning a random kick to the pitch-angle variable \( \xi = \tan(\nu_b/\nu_1) \). If the parallel and perpendicular velocity components of a given marker before the collision are designated \( v_{in} \) and \( v_{lin} \), respectively, and the initial value of the pitch-angle variable is \( \xi_{in} = \tan(\nu_b/\nu_{lin}) \), the following \( \xi \) becomes

\[ \xi_{out} = \left( \sin \Delta \theta \sin \varphi \sqrt{1 - \xi_{in}^2} + \xi_{in} \cos \Delta \theta \right), \]  

with \( \Delta \theta = R/2v\Delta T \) [28, 29]. In the previous expression \( \Delta T \) is the time-step, \( \nu \) the collision frequency as defined above, \( R \) a random number from a normal distribution function with expectation value zero and variance one and \( \varphi \) a random number from a uniform distribution between 0 and 2\( \pi \).

Taking \( f_0 = f_M \exp(-Ze_0\nu_0/T) \), as the solution of the zeroth order DKE,

\[ \frac{df_0}{dt} + v_1 \cdot \nabla f_0 - \left( \frac{\mu}{m_a}v_1 \nabla B + \frac{q}{m_a} \nabla \Phi_0 \right) \frac{\partial f_0}{\partial \nu_1} = C(f_0), \]  
(15)

with \( f_M = [m_0/(2\pi)^{3/2}] \exp[-(v_1^2 + v_T^2)/2] \) the standard local Maxwellian, equation (10) becomes,

\[ \frac{df_0}{dt} + \dot{R} \cdot \nabla f_1 + \frac{\partial f_1}{\partial v_1} = -f_0 (v_0 + v_{E1}), \]  

\[ \dot{R} = -\nabla f_0 \left[ \frac{n'}{n} + \frac{q}{T} \Phi_0 + \left( \frac{mv^2}{2T} - \frac{q}{2} + \frac{q}{T} \Phi_0 \right) \frac{T'}{T} \right] + C(f), \]  
(16)

where the species index has been dropped for convenience, the prime denotes the derivative with respect to \( r, v_{E1} = b \times \nabla \Phi_0/B \) is the \( E \times B \) drift related to the potential variation, and the \( \delta f \) part has been relabelled as \( f_1 \). Note that to derive equation (16) we have replaced (4)–(6) in (10) first, although we consider \( a \) posteriori the simplified characteristics (7)–(9) in the left-hand-side, i.e. in the integration of the marker trajectories. This implies the assumption that radially non-local terms, as well as terms involving the tangential components of the magnetic drift can be neglected when multiplying terms with \( f_1 \).
conditions that the magnetic configuration has to satisfy so that radially non-local terms can be dropped are identified in [30]. Neglecting the tangential components of the magnetic drift is correct as long as the $E \times B$ drift is sufficiently large. Finally note that in the present work $f_0$ differs from that in [21] where it was $f_M$, which means that $\Phi_1$ is kept as a first order magnitude for all species, including the impurities, in that reference. BlueApart from this $f_0 = f_M$ has the disadvantage that the flux driven by $f_0$ needs to be calculated as well, which afflicts the estimated flux with a strong numerical noise. This point is addressed in appendix B, where one of the LHD cases discussed below is considered in the discussion.

The solution of equation (16) when $\Phi_1$ is neglected leads to the same result as the standard mono-energetic and local neoclassical theory. In figure 1 a radial profile of the particle flux density for fully ionized carbon is presented, comparing results of EUTERPE and the 1D transport code NTSS [31, 32] which uses transport coefficients determined by DKES [33, 34]. Note that this benchmark case corresponds to the LHD magnetic configuration considered in section 3.1 for the case labelled as B.III and neglecting $\Phi_1$ (see figure 4).

2.2. Solution of the quasi-neutrality equation in EUTERPE

Regarding the electric field calculation the ambipolar part $\Phi_0$ is provided by the predictive transport code NTSS, mentioned at the end of the previous section. This code uses precalculated DKES mono-energetic coefficient databases that are, given a set of equilibrium profiles, appropriately convoluted to obtain the particle fluxes necessary for the ambipolar root-finding [31]. For the calculation of $\Phi_1$ performed with EUTERPE, instead of the less restrictive ambipolarly constraint the fulfilment of quasi-neutrality among all the species is required,

$$\sum_a Z_a e n_a = 0. \quad (17)$$

Considering the density up to first order in $\rho$, with the equilibrium part now varying on the flux surface due to the Boltzmann response

$$n_a = n_{0a} \exp(-Z_a e \Phi/T_a) + n_{1a} , \quad (18)$$

and assuming that $\sum_a Z_a e n_{0a} = 0$, when electrons, bulk ions, and one single impurity species with charge $Z$ are taken into account the following relation follows

$$\Phi_1 = T_e \left( n_{0e} + n_{0i} \frac{T_e}{T_i} + Z^2 n_{0Z} \right)^{-1} (n_{1i} - n_{1e} + Z n_{1Z}) , \quad (19)$$

and the exponent of the Boltzmann factor is assumed much smaller than unity for all species. For the calculations carried out in this work the electron response is assumed to be adiabatic and $f_{1e}$ is neglected since $f_{1e}/f_{1i} \sim \rho_e/\rho_i$ at comparable electron and bulk ion temperature. Since equation (19) is limited to the cases where $Z e \Phi/T_e \ll 1$, and this limit is questionable in situations with moderate to high $\Phi_1$ amplitude and $Z$, impurities are taken in this work at a sufficiently low concentration so that their influence on the potential can be neglected. The leap in complexity if more terms in the series must be retained or the Boltzmann response was kept in exponential form, leading to an equation non-linear in $\Phi_1$, is beyond the scope of the present work. Thus, under these assumptions the equation for $\Phi_1$ reduces to

$$\Phi_1 = \frac{T_e}{e} \left( n_{0e} + n_{0i} \frac{T_e}{T_i} \right)^{-1} n_{1i} , \quad (20)$$

and states that the potential that maintains charge quasi-neutrality at this order is exclusively due to the first order departure of the bulk ion density from its equilibrium value.

When solving equation (20) a low-mode-number filter is applied. In the present work poloidal and toroidal mode numbers $m$ and $n$ up to 4 have been sufficient to find good convergence of the calculated $\Phi_1$ and the related impurity fluxes. EUTERPE calculates $\Phi_1$ at each flux surface independently, which introduces a dependency on $r$ since $\Phi_1$ differs from one surface to another. Thus $\Phi_1$ over the simulation time is more properly expressed as $\Phi_1(r, \theta, \phi, t)$. Here $\theta$ and $\phi$ are the angular-like magnetic (PEST [35]) coordinates. The poloidal drift due to the radial variation of $\Phi_1$ will be ignored here since it is of the same order of magnitude as the tangential $\mathbf{b} \times \nabla \mathbf{B}$ component of $\mathbf{v}_s$ ignored when simplifying equations (4)-(7). The time dependency is averaged out during the time interval where stationary values have been reached within numerical error. For the remainder of this paper we will write the dependence of $\Phi_1$ as it is assumed and introduced as input for the impurity flux simulation: as a stationary potential $\Phi_1(\theta, \phi)$ which impurities do not influence given their low concentration. In figure 2 (left) an example of a $\Phi_1$ contour plot is presented. The corresponding complex Fourier coefficients are shown separately for the real and imaginary parts and appear normalised to the component with maximum amplitude, which in this case is the $\cos \theta$ term. Again note that the representation of $\Phi_1$ can be expressed as:

$$\Phi_1 = \sum_{m,n} [\mathcal{R}(\Phi_{1,mn}) \cos(m \theta + n \phi) + \mathcal{I}(\Phi_{1,mn}) \sin(m \theta + n \phi)] .$$

Finally the flux surface average $\langle \Phi_1 \rangle = \Phi_{1,00}$ must be zero since
is defined to be zero and the trajectories do not evolve radially due to the suppression of the drifts across the flux surface. Nevertheless this is not strictly the case and $\Phi_{1,00}$ usually develops some small finite value during the simulation, which is due to the numerical error accumulated in the integration of the trajectories and the presence of a small radial numerical drift. A low amplitude of the component $\Phi_{1,00}$ indicates a weak numerical departure from the exact trajectories and is correlated with tolerable noise situations, and filtering it out does not impact appreciably the calculation of any other quantity, including the radial flux of impurities. In figure 2 (right) such a situation is found where $\Phi_{1,00}$ is finite but nevertheless small. These figures are obtained for the case B.III discussed later in section 3.1. A benchmark of the calculations of $\Phi_1$ with the code SFINCS has recently been carried out and the results are presented in appendix A.

3. Radial flux of impurities including $\Phi_1$

In this section the numerical results are presented and discussed. Three different stellarator configurations, each from a different device type, have been considered: the large helical device (LHD, Toki, Japan) heliatron; the Wendelstein 7-X (W7-X, Greifswald, Germany) helias; and the TJ-II (Madrid, Spain) helicat. For each device a vacuum configuration has been considered and the radial particle flux of some representative impurities calculated, comparing the result when $\Phi_1$ is neglected to the result when $\Phi_1$ is retained. The scanned plasma parameters have resulted in 6 different pairs of density and temperature profiles for LHD, 5 for W7-X and 2 for TJ-II. The main parameters related to the three magnetic configurations are provided in table 1. The contour plots of the magnetic field modulus $B$ for the configurations considered are presented in figure 3.

3.1 LHD results

For LHD two different density profiles have been considered: one corresponding to a high-density scenario (A) and one corresponding to a low-density scenario (B). With respect to the temperature, three different bulk ion/impurity temperature profiles (I, II and III) have been considered, while the electron temperature has been kept constant throughout the present analysis. The density and temperature profiles are represented in figures 4(a) and (b), together with the ratio $a/L_a$ and $a/L_T$ for all species in figure 4(c), with $a$ the minor radius of the magnetic configuration and $L_Q = (\partial \ln Q / \partial r)^{-1}$ the radial variation length-scale of the quantity $Q$. Finally the ambipolar electric field is shown for the six resulting sets of profiles in figure 4(d).

Table 1. Major and minor radii, $R_0$ and $a$ respectively, and amplitude of the Boozer harmonic $B_{00}$ of the magnetic field at the mid plasma radius of the three configurations studied.

| Device        | $B_{00}(r/a = 0.5)$ (T) | $R_0$ (m) | $a$ (m) |
|---------------|--------------------------|-----------|---------|
| LHD           | 1.54                     | 3.6577    | 0.5909  |
| Wendelstein 7-X | 2.78                     | 5.5118    | 0.5129  |
| TJ-II         | 0.996                    | 1.5041    | 0.1926  |

Throughout this work a three species plasma has been assumed (hydrogen, electrons and one impurity species with charge $Z$). For the LHD results presented in this section fully ionised carbon $C^{6+}$ and neon $Ne^{10+}$ have been considered. The equilibrium density of the bulk ions $n_0$ and impurities $n_{0Z}$ is then initially taken so that quasi-neutrality among all the species at zeroth order is fulfilled. Thus $n_{0Q}(r) = n_{0Q}(r) [Z_{eff}(r) - 1] / [Z(Z - 1)]$ and $n_{0Q}(r) = n_{0Q}(r) [Z - Z_{eff}(r)] / (Z - 1)$. The reference value considered for the effective charge is taken in all cases to be $Z_{eff} = 1.1$ and it is held constant over $r$, which results in the bulk and impurity ion density profiles having the same shape as the electron density profile. Note that for all the LHD plasmas presented here $E_i$ is negative, and for the low-collisionality cases B, $E_i$ is relatively close to zero. The corresponding impurity inward pinch is then smaller than at higher collisionalities, which should make it easier for higher-order corrections to counteract the inward impurity pinch [36] as is shown below.

In figure 5 the normalised electrostatic potential $e\Phi_1(\theta, \phi)/T_i$ is presented for the three aforementioned ion temperature profiles I, II and III at the radial position $r/a = 0.6$. The three figures on the top correspond to the high-density cases A.I–III while the plots on the bottom correspond to the low density B.I–III cases. As the collisionality decreases and the temperature increases (following the six contour plots from left to
right and top to bottom) the normalised potential rises up to one order of magnitude from case A.I to B.III. Considering that \( \Phi_1 \) scales with the ion temperature, see equation (20), and that the collisions prevent the localised particles from completing their orbit and effectively contributing to \( \Phi_1 \), the trend that \( e\Phi_1/T_1 \) follows is qualitatively as expected.

Figure 6 shows the real and imaginary part of some representative Fourier coefficients of \( \Phi_i \). Note that for the real and imaginary parts filled and open points are used, respectively, while the point type is specific for the mode number, e.g. circles for \((m, n) = (1, 0)\). The typical values of the largest terms vary from a few volts of peak-to-peak potential variation in case A.I to around a hundred in case B.III. The change in the spectrum of the potential between the high density cases and the low density cases is appreciable too. At high density (top figures) the spectrum consists basically of two large \( \sin \theta \) and \( \cos \theta \) components of comparable size followed by other components appreciably lower in absolute value, among which the \( \cos 2\theta \) is the largest. On the other hand, the spectrum of \( \Phi_1 \) for the low-density cases (bottom figures) is characterised by a dominant \( \cos \theta \) component with no other component of similar prominence. In order to sketch what underlies these changes in the spectrum note first that \( \Phi_1 \), under the assumptions considered, reflects the same dependence as that of \( n_{\text{i1}} \), see equation (20), given by the perturbed distribution function of the bulk ions \( f_{1\text{i}} \). Regarding the dependence of the latter, and in particular the portion related to the ripple-localised particles which are largely responsible for \( \Phi_1 \), it is known for a classical stellarator \([16, 37]\) that in the asymptotic limit where the effective collision frequency exceeds the \( E_r \times B \) poloidal precession frequency \( (\Omega_{\text{B}} = E_r/rB_0 \ll \nu) \) the distribution function consists essentially of a \( \sin \theta \) component, while in the opposite rotational limit \( (\Omega_{\text{B}} \gg \nu) \) this becomes to a good approximation a \( \cos \theta \) term. In the cases presented, the parameters are such that \( \Omega_{\text{B}}/\nu \) take values from approximately 0.2 for the simulation with the highest ion collisionality (case A.I at \( r/a = 0.8 \)) to 20 at the lowest collisional one (case B.III at \( r/a = 0.8 \)). Thus qualitatively the changes in the Fourier spectrum of \( \Phi_1 \) can be reasonably well explained.

The question to what extent the radial impurity transport is affected by \( \Phi_1 \) has been addressed considering the potential calculated at four different radial positions for each set of profiles: \( r/a = \{0.2, 0.4, 0.6, 0.8\} \). The calculated potential at a given flux surface has been taken as an input for the estimation of the radial particle flux density \( \Gamma \cdot \nabla r \) of the impurity of interest. In figure 7 the results for LHD are shown. In all plots filled/open points correspond to the result including/neglecting \( \Phi_1 \). For better visualisation, points are connected by a solid/dashed curve respectively. The impurity species is denoted by a different point type and line colour. Fully ionised carbon and neon, \( C^{6+} \) and \( \text{Ne}^{10+} \), are represented with black circles and green diamonds respectively. The radial particle flux density is normalised to the equilibrium density value \( n_{\text{eq}} \) at each position. The electron density profile (A or B) and impurity temperature case (I, II or III) are indicated in the legend.

In a first overview of figure 7 and looking at the corresponding contour plots with the ratio \( e\Phi_1/T_1 \) shown in figure 5, for the two impurity species, a more significant change in the impurity fluxes is observed with increasing \( e\Phi_1/T_1 \).

Focusing on the high-density cases A, for the two impurity species the effect of the potential variation is initially found to be weak, see case A.I, and becomes more appreciable as the amplitude of \( e\Phi_1/T_1 \) (and the ion temperature) increases, see cases A.II and A.III. A large impact on the shape of the impurity flux profiles is not observed but mitigation of the inward flow does occur in the three cases for both carbon and neon.

We observe that for the low density cases B for the three species \( \Phi_1 \) has a much stronger impact on the radial flux than at high densities. Not only in absolute value but also in overall trend along the radial coordinate. Apart from the larger \( e\Phi_1/T_1 \) values the background plasma should not be overlooked [36]. For the low collisionality cases B the standard inward impurity pinch is smaller, and the correction caused by \( \Phi_1 \) makes a larger difference in the total impurity flux than in the cases without. Without \( \Phi_1 \) and regardless of the temperature profile (I, II or III) the radial flux of carbon monotonically becomes less negative with increasing \( r \). The effect of \( \Phi_1 \) reverses that tendency, leading to a stronger inward flow at the outer radii and a weaker one at the more inner positions. This loss of similarity between radial profiles with and without \( \Phi_1 \) is significantly more evident as \( \Phi_1 \) increases. Regarding the impact of the charge state, neon exhibits a slightly more pronounced change when \( \Phi_1 \) is considered than carbon does.

The underlying reasons that make the effect of \( \Phi_1 \) oppose or support the tendency of impurities to accumulate are difficult to deduce when comparing across cases and radial positions. The results indicate the necessity of a deeper quantitative look into the the problem, beyond the mere correlation between
parameters discussed so far, namely, potential amplitude, collisionality, charge state, etc.

To outline the intricate coupling that leads $\Phi_1$ to produce net particle transport note first that contrary to the magnetic field modulus $B$, $\Phi_1$ does not preserve the stellarator symmetry as it contains both cosine and sine components. This lack of stellarator symmetry arises indeed from the stellarator symmetry of $B$, which introduces only sine terms in the transport source $\dot{\rho} \cdot \nabla v_d$, which coupled to the cosine terms of $f_1$ vanish when the flux surface average operates on the particle-flux-density integral. Thus, the physical situation with non-zero radial transport requires $f_1$ to have sine components that, as discussed above, are the same for $n_{1Z}$ and $\Phi_1$. As a consequence, when $\Phi_1$ is taken into account and together with it $\dot{\rho} \cdot \nabla r$ as a transport source for the impurities, it is straightforward to recognise that this can drive radial transport through both sine and cosine components of $f_1$. How $\Phi_1$ affects the radial impurity flux requires knowledge about $f_{1Z}$, which $n_{1Z}$ captures only in truncated form due to the integration over velocity space. To illustrate this coupling, figure 8 shows an example of how the perturbed density and cross field drifts depend on $\Phi_1$. The figure refers to the carbon B.III case at the innermost radial position $r/a = 0.2$ (see bottom right plot in figure 7), which shows a reduction of the inward flux when $\Phi_1$ is present. The radial drifts for the two cases, magnetic $\dot{\rho} \cdot \nabla v_d$ (top left) and the sum of magnetic and electrostatic ($\dot{\rho} + \dot{\rho}_E) \cdot \nabla r$ (top right), are presented. For this example the thermal energy equally divided among the parallel and perpendicular kinetic energy has been considered for the drifts shown.

In the two bottom plots the density variations of carbon $n_{1C+}$ are represented for the case without $\Phi_1$ (bottom left) and for the case with $\Phi_1$ (bottom right). The contours of the radial drifts of the top figures are superimposed to the corresponding density contour plot for visualisation purposes. In the first of the density contour plots one can observe that the density exhibits an up-down pattern with low (high) density values around $\theta = \pi/2$ (\theta = 3\pi/2). The low density areas of the flux surface appear predominantly encompassed by contours of strong positive radial drifts while the high density regions coincide with those of negative drifts. This situation, which clearly supports the inward flow of carbon ions, is lost when $\Phi_1$ is present. In that case (see bottom right plot) a phase shift of $\pi/3 - \pi/2$ along $\theta$ in the carbon density, which becomes

![Figure 4. Radial profiles considered for LHD: (a) electron density; (b) electron, hydrogen and impurity temperature profiles; (c) minor radius $a$ normalised to the radial variation length-scale of density and temperature ($a/L_n$ and $a/L_T$); (d) ambipolar electric field $E_r$ obtained with NTSS for the resulting six combinations of ion density and temperature profiles.](image-url)
in–out asymmetric instead, leads the radial drift contour of largest outward and inward values to be both situated in the low density region located in between $\theta = \pi/2$ and $3\pi/2$. This does not support the enhancement of the inward pinch as was the case without $\Phi_1$.

### 3.2. Wendelstein 7-X results

In the present section a study similar to the one presented for LHD is carried out for the stellarator Wendelstein 7-X (W7-X). Profiles for this case are given in figure 9: electron density profile in figure 9(a); four different temperature profiles, equal
for all the species and labeled from I to IV in figure 9(b); to assist the interpretation of the fluxes below the radial profiles of $aL_a$ and $aL_T$ are shown in figure 9(c); and finally the radial ambipolar electric field $E_r$ provided by NTSS in figure 9(d). As before, the effective charge value $Z_{\text{eff}} = 1.1$ is considered constant along $r$, which defines the bulk and impurity ion density radial profiles.

The top row of figure 10 shows contour plots of the normalised electrostatic potential $e\Phi_1/T_i$ varying over the surface at the radial position $r/a = 0.6$. The values of $e\Phi_1/T_i$ calculated...
for W7-X are appreciably lower than for the LHD cases at comparable collisionality, which corresponds roughly to the high density cases A.I–III in figure 5 (top row) (a comparison of all simulation results is given in figure 18). The reason for the low value of the electrostatic potential in W7-X lies in the design of this device namely, reducing the neoclassical losses and bootstrap current by approaching an omnigeneous magnetic field structure. In a perfectly omnigeneous magnetic field the bounce-averaged drift surfaces of the localised particles coincide with the flux surfaces. Although this ideal situation cannot be exactly reached [38], the W7-X magnetic field structure is a better approximation than the other devices considered in this work, leading to a smaller departure of the localised particles from the flux surfaces and resulting in a weaker electrostatic potential variation on them. Regarding the Fourier spectrum of $\Phi_1$, similar features to LHD at comparable collisionality (cases A.I–III) are seen. A dominant $\sin \theta$ component and a weaker $\cos \theta$ that grows as collisionality decreases appear in both the W7-X and the LHD cases. On the other hand, the W7-X potential exhibits a broader spectrum, in the sense that the rest of the components are not as small—especially at the outer radii—as in LHD, where with the exception of $\cos 2\theta$ the remaining Fourier harmonics cluster around the value zero.

In figure 11 the particle flux density calculated for fully ionised carbon C6+ (circles) and Tungsten W40+ (triangles) is presented for the four ion temperature profiles in the top and bottom rows respectively. As before, filled (open) points linked with solid (dashed) lines correspond to the calculation including (neglecting) the potential variation on the surface. Looking at the carbon cases, the difference that $\Phi_1$ makes with respect to the standard neoclassical prediction is difficult to discern for the lowest temperature cases like I or II. As the ion temperature increases, in III and IV for instance, the impact becomes distinguishable and results in a weak mitigation of the inward radial flux. Nonetheless $\Phi_1$ makes little difference in the flux levels of these cases too. In the comparison for tungsten impurities shown in the bottom row of figure 11 the trend is the same, although the larger charge state makes the difference more clear between accounting for the potential variation and neglecting it, particularly in the lowest collisional cases III and IV.

As noted above, none of the cases I to IV is comparable in parameters (and collisionality) to the LHD low density set B.
which exhibits the most significant quantitative and qualitative change due to $\Phi_1$. Thus, in order to allow a comparison with those LHD cases an additional set of profiles for W7-X is presented. It corresponds to a W7-X plasma with off-axis ECRH where the density is lower than in the previous cases and the electron and ion temperature are comparable to the previous case IV. The same quantities as in figure 9 are represented for this case in figure 12: electron density in figure 12(a), electron and bulk/impurity ion temperature profiles in figure 12(b), $a/L_n$ and $a/L_T$ figure 12(c), and $E_r$ in figure 12(d). The contours of $e\Phi_1/T_e$ at the position $r/a = 0.6$ is presented in figure 13 (left) and the radial profiles of some of its Fourier harmonics of $\Phi_1$ in figure 13 (right). In this case the maximum potential amplitude is twice as high as in the previous case IV. The spectrum exhibits a very distinctive dependency on $r$, where no clear dominance of any component is present, except at the outer-most position where the components $\sin(\phi - \theta)$ and the $\sin \phi$ dominate.

Regarding the impurity radial fluxes, in the case of carbon (figure 14 (left)) the correction introduced by $\Phi_1$ is practically negligible. It is necessary to increase substantially the charge state, (see figure 14 right for a similar comparison for W$^{40+}$) to notice the difference. Here the inward pinch without $\Phi_1$ is barely zero ($r/a = 0.2$ and 0.4), due to the low negative $E_r$ values (see figure 12 (right)). And the introduction of $\Phi_1$ leads the inward pinch to become appreciable. Anyhow, the difference between the case without and with $\Phi_1$ is still not larger than in case IV discussed above, despite the increase of $e\Phi_1/T_e$ by a factor of two. This lack of response to a larger $e\Phi_1/T_e$ may indicate again that the specific coupling between the potential variation and the distribution function $f_1$ is playing a role, as the discussion at the end of section 3.1 already noted. This represents an entire topic to look deeper into in another work.

3.3. TJ-II results

Finally in the present section two cases are considered for the TJ-II stellarator. Two electron density profiles (high and low density) shown in figure 15(a) have been considered, with the temperature profiles for the electrons, bulk ions and impurities given in figure 15(b). The corresponding profiles of $a/L_n$ and

Figure 9. Plasma parameters considered for W7-X: (a) electron density; (b) temperature profiles I to IV with $T_e = T_i = T_s$ in each case; (c) minor radius over the variation length-scale of density and temperature ($a/L_n$ and $a/L_T$); (d) ambipolar electric field $E_r$ obtained with NTSS for the four cases considered.
and the ambipolar electric field profiles of the two cases are given in figures 15(c) and (d) respectively. The impurities considered are fully ionised carbon C6+ and partly ionised tungsten W15+. These profiles correspond to typical NBI-heated TJ-II plasmas [39, 40].

In figure 16 (top) the normalised electrostatic potential \( \Phi_1 \) is plotted at the radial position \( r/a = 0.6 \) for the high- and low-density cases. The amplitude of some representative Fourier harmonics (bottom) are also shown. Looking at the latter figure the harmonics of \( \Phi_1 \) are lower in amplitude than LHD and of the same order of magnitude as in the W7-X cases, of a few volts. Nevertheless, the much lower ion temperature of these TJ-II examples indeed represents the largest ratio \( \Phi_1 \) at comparable collisionality of the three devices studied—see figures 5 (top) and 10 (top) for the same quantity represented for LHD and W7-X similar collisionality cases. Further discussion comparing all the cases studied in this work is provided in section 4, but we note already in this section that the electrostatic potential energy related to \( \Phi_1 \) can vary (considering thermal bulk ions) up to 5–8 % in terms of kinetic energy for the high density TJ-II case and up to 10–15 for the low density one. For LHD and W7-X the variation is respectively one and two orders of magnitude lower than that. In contrast to W7-X, where the neoclassical optimisation explains the weak \( \Phi_1 \), the lack of such optimisation in TJ-II and much larger effective ripple (see [10]) supports large potential variations like those calculated here and observed experimentally [41].

The results for the radial impurity flux are presented in figure 17 for the high/low density cases in the two figures on the left/right, and for the two species considered, C6+ on top and W15+ on the bottom. The radial impurity transport is not...
Figure 12. Radial profiles for the W7-X case with off-axis ECRH: (a) electron density; (b) electron, bulk ion and impurity temperature; (c) minor radius over the variation length-scale of density and temperature ($a/L_n$ and $a/L_T$); (d) ambipolar electric field $E_r$.

Figure 13. Electrostatic potential variation at $r/a = 0.6$ and some representative Fourier harmonics of $\Phi_1$ as a function of $r/a$ for the W7-X case with off-axis ECRH.
Figure 14. Radial particle flux density of C$^{6+}$ (left) and W$^{40+}$ (right) as a function of $r/a$ including $\Phi_1$ (filled dots linked with solid line) and neglecting it (open dots linked with dashed line) for the W7-X case with off-axis ECRH.

Figure 15. Radial profiles for the TJ-II cases: (a) electron high and low density cases; (b) electron, bulk ions and impurity temperature; (c) minor radius over the variation length-scale of density and temperature ($a/L_n$ and $a/L_T$); (d) ambipolar electric field $E_r$. 
affected by the presence of $\Phi_1$ to the extent its large amplitude for such low temperatures might lead one to expect. It does not differ qualitatively from the standard neoclassical prediction, although quantitatively the changes observed in the flux are appreciable and tend to decrease the inward flux. Note the similar values of $C_i^{\phi}$ normalised radial flux to those reported in [42]. The impact for carbon and tungsten is also comparable despite the different charge states. This weak response to relatively large values of $\Phi_1$ and charge state again points out to the fact that the impact of $\Phi_1$ on the radial transport cannot be explained only with the size of the parameters under discussion. As noted at the end of section 3.2 and more in detail in section 3.1, the spatial dependence of $f_{1Z}$ depends on these parameters too and changes from case to case, and with it, the coupling with $\Phi_1$ to finally impact the radial transport more or less efficiently. Finally, regarding the spectrum of $\Phi_1$ shown in figure 16 (bottom), TJ-II exhibits several large terms, among which the $\cos \theta$ term and the helical components $\cos(\theta + \phi)$ or $\sin(\theta + \phi)$.

4. Final remark on the amplitude of $\Phi_1$ in LHD, W7-X and TJ-II

The smallness of $Ze\Phi_1/T$, as was noted in the introduction, indicates the reliability of the standard neoclassical neglect of $\Phi_1$ as source of trapping and radial transport of impurities. Taking $\Delta \Phi_1$ to be the maximum potential variation on a flux surface, $e\Delta \Phi_1$ is the total energy variation that a bulk ion, or impurity if multiplied by $Z$, can experience on a flux surface due to $\Phi_1$. In order to compare all the cases and configurations considered here, figure 18 shows the ratio $e\Delta \Phi_1/T$ as a function of the bulk ion normalised collisionality, $\nu_0 = \nu_eT_0/\nu_iT_i$, where $\nu$ is the rotational transform. The figure takes into account the four radial locations considered for each set of profiles and devices considered in the present paper.

From this representation it is clear that assuming monoenergetic trajectories for impurities often becomes questionable and the effect of $\Phi_1$ (as confirmed in the simulations presented) can be important in LHD and TJ-II. In these two devices the electrostatic energy variation normalised by the thermal energy exceeds at most radial positions and in most
cases the level of a few percent (and in some cases ten percent). This ratio appropriately scaled by a moderate to large impurity charge (and at some positions also by a low charge) becomes of order unity. This is clearly the case for the low-density set of LHD profiles B.I–III and the two TJ-II cases. TJ-II exhibits potential variations of the order of those given in LHD for the B set of profiles at much lower collisionality. At a comparable range in collisionality, LHD cases A.I–III develop a $\Phi_1$ roughly an order of magnitude lower than TJ-II. Similarly, comparing W7-X and LHD, the former device has values of $\Delta \Phi_{eT}$ one order of magnitude lower than comparable cases for the latter.

For the W7-X cases studied, the ratio on the other hand takes maximum values of around and slightly below one percent, which may result in a moderate impact on highly charged impurities like tungsten, but has a negligible effect on the radial transport of low charge impurities like carbon.

Finally, the quantitative impact of $\Phi_1$ and the conclusions drawn from the cases considered in this work should be taken cautiously when extrapolating them to parameters distant from the present ones, as they follow from a limited set of profiles. In addition, the changes in the impurity distribution function $f_{iZ}$, and hence in the density of impurities $n_{iZ}$, are noted to play a role from the fact that in a few examples the

Figure 17. Radial particle flux density of $C^{6+}$ (top) and $W^{15+}$ (bottom) as a function of $r/a$ including $\Phi_1$ (filled dots linked by solid lines) and neglecting it (open dots linked by dashed lines), for the high and low density TJ-II cases (left and right respectively).

Figure 18. Normalized maximum variation of the potential $e\Delta \Phi_{eT}/T$ for all the cases presented in this work, as a function of the normalised thermal collision frequency $\nu^*$.
impact is weaker than what one would expect from the magnitude of $e\Delta \Phi_1/T$.

5. Summary and conclusions

The radial transport of impurities is known to be strongly influenced by the ambipolar part of the electrostatic potential, usually considered as an approximation to the full neoclassical electrostatic potential. In the present work, we have also taken into account the potential variation on the flux surface $\Phi_1$ found by solving the quasi-neutrality equation. The impact of $\Phi_1$ on the radial particle flux of a few impurity species in the devices LHD, W7-X and TJ-II, using the code EUTERPE has been presented considering some typical plasma profiles.

The calculations have to a varied extent confirmed the importance of taking $\Phi_1$ into account to quantitatively assess the radial transport of impurities. In LHD the effect of $\Phi_1$ was visible in all cases, and in the low collisional ones strong corrections in the radial flux profiles have been shown, including both the mitigation and enhancement of the inward flux. In typical TJ-II NBI-heated plasmas including the role of $\Phi_1$ has resulted in appreciable change as well, although weaker than what could be expected from the large potential variation predicted for this device.

Finally, in W7-X $e\Phi_1/T$ has been found roughly to be one order of magnitude lower than in LHD and nearly two orders below TJ-II. Low charge impurities like C$^{6+}$ are thus unaffected by $\Phi_1$ but highly charged impurities like W$^{40+}$ could experience some moderate change in their fluxes.

Apart from a more exhaustive parameter and magnetic configuration scan, some issues remain open, namely: study of the specific coupling between $n_{it}$ and $\Phi_1$ which may result in scenarios with little or no impurity accumulation; the relaxation of the tracer impurity limit since accumulation unavoidably leads to appreciable impurity concentrations; relaxation of the assumption of an electron adiabatic response whenever meaningful.

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Appendix A. Benchmark between EUTERPE and SFINCS

SFINCS [23, 43–46] is a 4D drift-kinetic equation solver for computing radially local neoclassical phenomena in non-axisymmetric plasmas. The code can be run with an arbitrary number of kinetic plasma species, and it implements the full linearized Fokker–Planck–Landau operator for self- and inter-species collisions. Numerically, it uses continuum methods, with finite differences in the two spatial coordinates (poloidal and toroidal angles $\theta$ and $\phi$), and spectral methods in the two velocity coordinates (normalized speed $x = v/v_0$ and pitch-angle $\xi = \psi/v$). SFINCS has recently been updated to account for the flux-surface variation of the electrostatic potential, solving a system that is nonlinear in the unknowns, $f_i$ and $\Phi_1$. The system that is solved includes the drift-kinetic equation, the quasi-neutrality equation, and a set of additional constraints for the unknowns. These constraints have been added, in conjunction with introducing particle and heat sources in the drift-kinetic equation, to enable a steady-state solution to exist (see [23, 43] and for additional details).

In the present work we use the same quasi-neutrality equation in SFINCS as in EUTERPE, the electrons are assumed adiabatic and impurities are neglected, and we do our calculations with the pitch-angle scattering operator. However, it should be noted that there are three differences compared to the EUTERPE implementation: Firstly, even though the impurities are neglected in the quasi-neutrality condition the whole system is still solved simultaneously which implies that it is still nonlinear (i.e. $\Phi_1$ is not given as a direct input to the kinetic equation of the impurities). Secondly, in the kinetic equations of both the main ions and the impurities SFINCS neglects collisions with the adiabatic electrons. And third in SFINCS there is no Fourier-filtering of $\Phi_1$, that is, $\Phi_1$ is stored with the same $\theta$ and $\phi$ resolution as $f_i$. The numerical resolution which is required for convergence in SFINCS depends strongly on the magnetic geometry and the collisionality. In the long mean-free-path regime the number of grid points required in $\theta$, $\phi$ and $\xi$ can increase dramatically as the collisionality decreases. Since the time and memory requirements increase significantly when more grid points are used, it is often desirable to use an individual resolution at each radius which is analyzed. The minimum resolution used in any of the SFINCS runs is $N_\theta = 43$, $N_\phi = 59$ grid points in the poloidal and toroidal direction (per identical segment of the stellarator), $N_\xi = 96$ Legendre polynomials to represent the distribution function and $N_t = 10$ grid points in energy.

The comparison between the calculation by SFINCS and EUTERPE of the electrostatic potential $\Phi_1$ is presented in figure A1. The case considered in this benchmark is the one labelled as A.III in section 3.1 for LHD, and taking the radial positions $r/a = \{0.2,0.4,0.6,0.8\}$ (displayed from left...
Slight differences are observed between the contour plots, which can be attributed to the differences noted above. On the other hand, the absolute value of the potential is in good agreement. In any case, the disagreement is not such that the values of the radial particle flux of carbon C$_6^+$ obtained by both codes deviate from each other. This is what Figure A2 shows, where the circles with error bars show the calculation with EUTERPE and the stars show the results with SFINCS. As in previous figures, filled points and solid lines refer to the case including $\Phi_1$ while open points and dashed lines indicate the standard calculation without it.

**Appendix B. Comparison of the impurity fluxes for different $f_0$ choice**

In the present work the choice of the background distribution function differs from that in [21]. Nevertheless, the different equations for the drift kinetic equation for the $\delta f$ part, expression (11) in [21] and (16) in this work, provide similar results although the one chosen here has the advantage that it suffers less numerical noise. The adoption of $f_0 = f_M \exp(-Ze\Phi_1/T)$ instead of $f_0 = f_M$ presents the feature that the radial flux driven by $f_0$ is zero when $\Phi_1$ is taken into account:

$$\left\langle \int \frac{1}{\sqrt{E}} \left( \frac{\partial F}{\partial \varphi} + J \frac{\partial F}{\partial \theta} \right) \right\rangle = 0,$$  \hspace{1cm} (B.1)

with $\langle \ldots \rangle$ the flux-surface-average operator and $\psi$ the flux surface label. To demonstrate relation (B.1) the stellarator magnetic field using Boozer coordinates $\psi, \vartheta, \varphi$ is considered: $B = I(\psi) \nabla \theta + J(\psi) \nabla \varphi + K(\psi, \vartheta, \varphi) \nabla \psi$. For any scalar field $F(\psi, \vartheta, \varphi)$ one has that $(B \times \nabla F) \cdot \nabla \psi = D(F)$ where $D$ is the operator

$$D(F) = \frac{1}{\sqrt{E}} \left( \frac{\partial F}{\partial \varphi} + J \frac{\partial F}{\partial \theta} \right),$$  \hspace{1cm} (B.2)

and $\sqrt{E} = |(\nabla \psi \times \nabla \varphi) \cdot \nabla \psi|$ is the Jacobian. Recalling that the drift velocities can be written as $v_d = (m/q)(v_d^2 + \mu_B)B \times \nabla \psi/B^2$ and $v_{EI} = B \times \nabla \Phi_1/B^2$, substituting into (B.1) and integrating in velocity yields

$$\left\langle \int \frac{1}{\sqrt{E}} (v_d + v_{EI}) \cdot \nabla \psi f_M \exp(-Ze\Phi_1/T) \right\rangle \propto \left[ \frac{T}{q} \int \frac{d\psi d\vartheta d\varphi}{B^2} \exp(-q\Phi_1/T) \right],$$  \hspace{1cm} (B.3)

that vanishes since the integrand on the right consists of derivatives with respect to the variables of integration of a function that is periodic on those variables. A similar argument applies to

$$\left\langle \int \frac{1}{\sqrt{E}} (v_d + v_{EI}) \cdot \nabla \psi f_M \right\rangle = 0,$$
because \( \int d^3v (\psi \cdot \nabla \psi) f_0 \) is generally different from zero. This last contribution to the flux which was neglected in [21] is included in the following comparison. In figure B1 the total flux of carbon for the B.III LHD case at \( r/a = 0.6 \) is presented along the simulated time, showing separately the contribution to the flux driven by \( f_0 \) and \( \delta f \). The left plot corresponds to the case \( f_0 = f_M \) and equation 11 of [21] while the right plot refers to the choice \( f_0 = f_M \exp(-q\Phi_1/T) \) and equation 16 of this work. As demonstrated \( f_0 = f_M \exp(-q\Phi_1/T) \) leads to a flux that is on average zero and hence the diagnosed total flux can be obtained as a moment of the small \( \delta f \) part and consequently exhibits a more benign numerical noise. It can be noted that the flux driven by \( \delta f \) in this right plot converges to approximately the sum of the two represented in the left plot.

This is more evident in figure B2 which shows the comparison of the flux between the two \( f_0 \) choices as a function of \( r/a \). It can be observed that the only discrepancy relates to the error-bar size. Although 10 times as many markers were loaded for the simulations where \( f_0 = f_M \) than for \( f_0 = f_M \exp(-q\Phi_1/T) \) (\( N_m = 3 \times 10^7 \) and \( 3 \times 10^6 \), respectively) the error-bar is still smaller in the second case. There are no further difference in the method applied in [21] and in this paper except those that the choice of \( f_0 \) implies. These are that the markers in the impurity cases where \( \Phi_1 \) is considered must be initialized with the corresponding Boltzmann response when \( f_0 = f_M \exp(-q\Phi_1/T) \). And as already pointed out the drift kinetic equation solved is equation (11) in [21] when \( f_0 = f_M \) and equation (16) when \( f_0 = f_M \exp(-q\Phi_1/T) \). The approximations in both works are the same: adiabatic electron response, tracer impurities, and neglect of the magnetic and \( \times \mathbf{E} \times \mathbf{B} \) drifts to lowest order in \( \rho_e \) in the marker trajectories, i.e. on the left-hand-side of the drift kinetic equation.

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