Neoclassical flows in deuterium–helium plasma density pedestals

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Abstract
In tokamak transport barriers, the radial scale of profile variations can be comparable to a typical ion orbit width, which makes the coupling of the distribution function across flux surfaces important in the collisional dynamics. We use the radially global steady-state neoclassical \(\psi\) code PERFECT (Landreman et al 2014 Plasma Phys. Control. Fusion 56 045005) to calculate poloidal and toroidal flows, and radial fluxes, in the pedestal. In particular, we have studied the changes in these quantities as the plasma composition is changed from a deuterium bulk species with a helium impurity to a helium bulk with a deuterium impurity, under specific profile similarity assumptions. In the presence of sharp profile variations, the poloidally resolved radial fluxes are important for the total fluxes to be divergence-free, which leads to the appearance of poloidal return-flows. These flows exhibit a complex radial–poloidal structure that extends several orbit widths into the core and is sensitive to abrupt radial changes in the ion temperature gradient. We find that a sizable neoclassical toroidal angular momentum transport can arise in the radially global theory, in contrast to the local.

Keywords: neoclassical transport, tokamak, radially global, pedestal, flows, deuterium, helium

(Some figures may appear in colour only in the online journal)

1. Introduction
Transport barriers are regions in a magnetically confined plasma with reduced cross-field turbulent transport, which leads to steep gradients in density and temperature. Such formations have a major impact on fusion plasmas, as they can enable fusion relevant conditions to be reached in smaller devices. Thus, practically all plans for future magnetic fusion experiments and reactors include at least an edge transport barrier, commonly known as the pedestal.

Since the discovery of transport barriers (the ELMy H-mode [1]) there have been numerous studies [2–6] indicating the crucial role plasma flows play in the transition to improved confinement regimes. In particular, the equilibrium flows have been experimentally observed to play a major role in setting the transition threshold [7]. Thus well resolved plasma flow measurements in the pedestal, especially those of the main ion species, are highly desirable for progress in the understanding of the barrier formation.

However, the flows of fusion relevant hydrogen ions are challenging to infer directly due to their involved emission spectrum, which complicates the use of standard charge exchange techniques (see [8] for a recent effort to tackle these difficulties in DIII-D). Instead, flow diagnostics often rely on measuring the flows of some impurity species, such as He [9], B [10] and C [9, 11], from which the deuterium flows are inferred. Yet another technique is to measure the main ion flows in non-hydrogenic plasmas; this approach has been used with helium plasmas, in DIII-D [12], and recently in ASDEX Upgrade [13].

That being said, theoretical calculations are required to relate these flows to deuterium flows. Specifically, it is important to know how impurity ion flows relate to main ion flows, and how the flows in helium and deuterium bulk plasmas compare to each other. These questions have previously been addressed with local neoclassical predictions [14, 15]. Such local calculations assume a scale separation between the radial variations in plasma profiles and the orbit width, thus they are not necessarily applicable to the H-mode
pedestal, where profiles can vary significantly over an orbit width. It is in the pedestal where flow measurements would be particularly interesting in order to study the H-mode, and neoclassical effects may be expected to contribute most strongly as a result of the reduced turbulent transport.

To address these questions in relation to the pedestal, we numerically investigate neoclassical flows in deuterium and helium plasmas, using the neoclassical global $\delta f$ code PERFECT (pedestal and edge radially-global Fokker–Planck evaluation of collateral transport) [16, 17]. The model profiles used here follow the approach of [18] to capture features of experimental JET pedestals [19] in multi-species simulations, while remaining within the validity of the $\delta f$ theory.

Due to the radial coupling in the global theory, the resulting fluxes are not divergence free within flux-surfaces. Thus flows within flux surfaces should be considered together with the radial flows. This has been considered as an explanation for poloidal impurity flow observations in [20], although modeling of the radial–poloidal flow structures was outside the scope of their study. In this paper, we discuss radial transport alongside poloidal and toroidal flows.

In section 2, we describe the radially global $\delta f$ theory, including constraints posed by our linearization about a Maxwell-Boltzmann distribution. In section 3, we relate the assumptions presented in the previous section to design choices in our numerical study, and present two bulk helium scenarios based on different similarity assumptions. Flows in both local and global simulations are presented, and we find that the global poloidal flows display notably larger poloidal and radial variations, with odd-parity in–out structure, which is sensitive to changes in the temperature gradient. Poloidally resolved radial flows are then considered together with poloidal flows. Finally, we consider the total radial transport of particles, heat and toroidal angular momentum. In global simulations we observe order unity modulations to the local and global $\delta f$ flows. This has been considered as an explanation for poloidal impurity flow observations, while remaining within the validity of the $\delta f$ framework.

Defining the non-adiabatic part of $f_i$ as

$$g = f_i - \frac{Ze\Phi_i}{T}f_M,$$

we linearize (1) to obtain

$$(v_i b + v_0) \cdot (\nabla g)_{W_0,\mu} - C_1[g] = -v_m \cdot (\nabla f_M)_{W_0,\mu},$$

where $C_1$ is the linearized Fokker–Planck operator, $W_0 = m v_0^2/2 + Ze\Phi_0$; $\Phi_1$ has been eliminated from the drift velocity $v_0 = B \times B \times \nabla \Phi_0 + v_m$ and we have assumed a steady state distribution, $\partial f / \partial t = 0$.

We are now in a position to more precisely define our expansion parameter $\delta$. By construction, $g f_M = O(\delta)$, thus $\delta$ measures the size of $g$. The size of $g$ scales with the inhomogeneous term on the right-hand side of (3), which can be approximated as [17]

$$v_m \cdot (\nabla f_M)_{W_0,\mu} = v_m \cdot \nabla \psi \frac{\partial}{\partial \psi} \left[ \left( \frac{m}{2T} \right)^{3/2} \eta_0 e^{w_0} \right],$$

where $W_0$ is a constant with respect to our derivative, and we have introduced the pseudo-density

$$\eta_0(\psi) = n_0 e^{Ze\Phi_0/Tc}.$$

(Henceforth, to streamline notation, the subscript ‘0’ will be dropped.) It follows from (4) that only the temperature and $\eta$ gradients enter into the inhomogeneous term in (3) and thus set the size of $g$ and act to make the distribution function non-Maxwellian. To characterize the size of the gradients of $\delta f$...
plasma parameter $X$ we introduce

$$\delta_X \equiv \frac{\rho_p}{L_X},$$  \hspace{1cm} (6)$$

where $\rho_p = mv_T/(Z e B_p)$ is the poloidal gyroradius, with the poloidal magnetic field $B_p$, and thermal velocity $v_T = \sqrt{2T/m}$; and $L_X = -[d(\ln X)/dr]^{-1}$ is the scale length of $X$. Since the size of the departure from $f_M$ depends on the gradients in $\eta$ and $T$, we can finally give a conservative definition of our expansion parameter $\delta$ as

$$\delta = \max_{\psi X} \delta_X(\psi) \ll 1,$$  \hspace{1cm} (7)$$

where $a$ is a species index. In words, $\delta$ is the largest value of the $\delta_X$ profiles corresponding to $T_e(\psi)$ and $\eta_p(\psi)$, among all species.

Note that while $n$ and $\Phi$ can vary on shorter length scales if the corresponding $\eta$ has a slow radial variation, the DKE (1) itself is based on an expansion in $\rho/L_X = (B_p/B)\delta$ for all plasma parameters, so no plasma profile may have gyroradius scale variation. We also require $B_p/B \ll 1$ to ensure that the gyroradius and the orbit-width expansions can be performed separately.

Equation (3) is the global linearized DKE, from which the conventional local $fi$ equation can be recovered by dropping the $v_B \cdot \nabla g$ term. The latter is solved when we refers to ‘local’ solutions. This corresponds to ordering $\nabla g = O(\delta f_M/L)$, meaning that the radial variation of $g$—and thus the radial variation of radial fluxes [16]—appear at order $(B_p/B)\delta^2 m v_T/L$ in (3). Note that neglecting $v_B \cdot \nabla g$ means that $\psi$ only appears as a parameter in the local equation, while the global equation is a differential equation in $\psi$, and thus requires radial boundary conditions. (In this work, we use solutions to the local equation as boundary conditions; see the first part of section 3 for details.)

In the pedestal region, $v_{x0} \cdot \nabla g$ must be retained, as the radial variation of the fluxes is in general not small in the presence of sharp background profiles. However, radially varying steady-state particle fluxes are inconsistent with particle conservation, unless they are compensated for by sources in the DKE (3) [16].

These sources may represent real sources, due to atomic physics processes, but could also include the radial variation of other fluxes—due to e.g. turbulence—which are excluded from our modeling but needed to cancel the radial variation of the modeled fluxes. We thus add a source term $S$ to (3) and obtain

$$(v_B + v_{x0}) \cdot (\nabla g)_{x,\psi} - C_1 g = -v_m \cdot (\nabla f_M)_{x,\psi} + S,$$  \hspace{1cm} (8)$$

which is the equation we solve when we refer to ‘global’ solutions.

The velocity and poloidal dependence of the sources are specified to yield particle and heat sources, while the radial dependence of these sources is solved for alongside $g$ by imposing that the perturbed distribution function should have zero flux-surface averaged density and pressure. This means that the input profiles specify the flux surface averages, that is $X_0 = \langle X \rangle \equiv (\psi')^{-1} \int X |B \cdot \nabla \theta|^{-1} d\theta$, \hspace{1cm} (9)

$$V' \equiv \oint |B \cdot \nabla \theta|^{-1} d\theta,$$  \hspace{1cm} (10)$$

where $\theta$ is an angle-like poloidal coordinate, and we introduced the flux surface average, denoted by $\langle \cdot \rangle$. In this work, we assume that the sources have no poloidal dependence, and have the same velocity structure as in [17].

3. Simulations and results

We consider a plasma with deuterium as bulk species and helium as impurity, and a bulk helium plasma with a deuterium impurity species, as two extreme cases of an ion concentration scan.

We would like to focus on differences in neoclassical phenomena that are linked to the charge and mass of the various ion components; our philosophy is thus to minimize changes in the plasma profiles as the ion composition is changed. In reality, plasma with different ion composition can have significantly different profiles, for reasons ranging from basic physical differences related to mass and charge dependences of various phenomena [28] to more practical ones, such as differences in heating or recycling [29].

Focusing these complications, we consider two scenarios, with profiles based on different similarity assumptions, which we refer to as fixed $\Phi$ and fixed $n_e$. The different names indicate which profile in the quasi-neutrality condition,

$$n_e = Z_D\eta_D e^{-Z_{He} e \Phi/T_{He}} + Z_{He}\eta_{He} e^{-Z_{He} e \Phi/T_{He}},$$  \hspace{1cm} (11)$$

is kept fixed when changing from a D to He bulk plasma. It is convenient to express this relation in terms of the ion pseudo-densities and temperatures, as these are constrained by (7).

For the ion pseudo-density profiles we use linear profiles, with a slope based on the experimental JET outer core $n_e$ profile of figure 16 in [19]; these core gradients generally satisfy the constraints posed by (7). Likewise, our ion temperature profiles were based on the core temperature gradient of the same figure. In addition, we further reduce the ion temperature gradients in the core to make a proxy for the local deuterium heat flux, $Q_D \sim n_D T_D^2 \partial_r T_D$, equal to the boundaries. This change in gradients both reduces the total heat and particle sources, when integrated over the simulation domain, while it also leads to a localization of sources around the pedestal region [17]. We will discuss the effect of changes in the temperature gradient in section 3.1.1.

The electron temperature profile is allowed to have structure on the ion orbit width scale, and thus uses the full temperature profile in figure 16 of [19]. We note that, as a consequence, the electron flows are much larger than the ion flows in absolute magnitude, and thus the bootstrap current is dominated by the electron contribution. As a result, the fixed $n_e$ similarity class keeps the bootstrap current profile practically fixed.

In the fixed $\Phi$ scenario, $\Phi$ is then chosen to make $n_D$ similar to the experimental $n_e$ profile. Finally, $n_{He}$ is determined by $\Phi$, $T_{He}$ and $\eta_{He}$. Bulk D and He plasmas are
obtained by rescaling the ion $\eta$ profiles relative to each other, which yields electron density profiles that vary with the ion concentrations—while leaving $\delta_n$ unaffected. Although the shape of $n_e$ varies, the ion profiles are re-scaled to yield the same electron density at the pedestal top.

In the fixed $n_e$ scenario, $n_e$ is instead specified from the experimental $n_e$ profile, and $\Phi$ is obtained from the quasi-neutrality condition (11), and thus depends on the helium concentration. Note that for a pure deuterium plasma, the methods yield the same electron density pro-

The pedestal usually extends outside the last closed flux surface (LCFS), while our model is restricted to closed field lines. We consider the region which would be in the open field line region as a numerical buffer region of the simulation. Such a region is introduced to better accommodate the outer radial boundary condition imposed in the simulation: a solution to the local DKE is imposed as boundary condition for both $\phi$ and $n_e$, and the bulk deuterium simulations are approximately the same in both similarity classes.

The resulting input profiles are depicted in figure 1, for the fixed $\Phi$ and fixed $n_e$ scan (left and right columns, respectively). In both scans the blue profiles are for bulk-deuterium plasmas ($n_{He}/n_D = 0.01$ in the core region) and red lines are for bulk-helium plasmas ($n_D/n_{He} = 0.01$); solid lines are electron profiles, dashed lines are deuterium and dash-dotted lines helium. As a radial coordinate we use

$$\psi^\circ = \psi - \psi_{LCFS}$$

which is the poloidal flux normalized and shifted so that $\psi^\circ = 0$ at the LCFS and a unit change of $\psi^\circ$ corresponds to a typical trapped thermal deuterium orbit width at $\psi = \epsilon$ is the inverse aspect ratio (defined as in Miller geometry [30]). The last subfigures in figure 1 depict the species self-collisional-

$\nu_{\alpha\alpha} = \frac{\nu_{\alpha\alpha}}{v_T/qR_0} = qR_0 \frac{Z^2}{12\pi^{1/2}} \frac{\epsilon^2}{e^2} T_{n\alpha}^2$.

In the following figures, curves are color coded as in figure 1 to indicate ion composition. In addition, dashed lines indicate output from local simulations, and solid lines are global results. The same color and line styles are applied to the frames of 2D plots. The following normalization is used throughout the paper. Quantities with a hat are normalized to a reference quantity that is species-independent in most cases, $X = X/\bar{X}$. The reference quantities used in this work are: $\bar{R} = 3.8 \text{ m}$, $\bar{B} = 2.9 \text{ T}$, $\bar{n} = 10^{20} \text{ m}^{-3}$, $\bar{T} = e\Phi = 1 \text{ keV}$, $\bar{m} = m_D$, where $m_D$ is the deuterium mass. These numbers are based on ‘typical’ quantities for JET, and only affect the normalization of the results. From these, we define a reference speed as $\bar{v} = \sqrt{2T/\bar{m}}$, and the dimensionless constant $\Delta = m\bar{v}/(e\bar{B}\bar{R})$, which corresponds to a normalized gyroradius at the reference quantities. Specifically, we have: fluid flow velocity $\bar{V} = V/(\Delta \bar{v})$; sources $\bar{S} = \epsilon^2 \bar{R} \bar{S}/(\Delta \bar{v}^2 \bar{m})$; flux surface incremental volume $\bar{V}^\prime = (\hat{\bar{B}}/\bar{R}) d\bar{V}$, particle flux, $\bar{f}_a = \int d^2\nu_{l\alpha \alpha} n_{l\alpha \alpha}/(\bar{\nu} \bar{m})$; toroidal momentum flux (divided by mass), $\bar{P}_l = \int d^2\nu_{l\alpha \alpha} \bar{v}_l n_{l\alpha \alpha}/(\bar{\nu}^2 \bar{m} \bar{R})$, with $I(\psi) = \bar{R}_l \bar{R}$ the major radius and $\bar{R}_t$ the toroidal magnetic field; heat flux, $\bar{Q}_a = \int d^2\nu_{l\alpha \alpha} m_{l\alpha \alpha} \bar{v}^2 n_{l\alpha \alpha}/(2 \bar{T} \bar{\nu} \bar{m})$; conductive heat flux, $\bar{q}_a = \bar{Q}_a - (5/2) \bar{\bar{\bar{B}}} \bar{I}_a'$. In addition, we define the normalized scalar radial particle flux

$$\bar{f}_a = \frac{\bar{V}^\prime}{\Delta \bar{R} \bar{B}} (\hat{\bar{I}}_a \cdot \nabla \bar{\psi})$$

and analogously, scalar fluxes for heat and momentum. When comparing poloidal and radial fluxes (as in figure 6), it is convenient to instead project the radial fluxes on a unit vector, in which case we use $\bar{I}_a \cdot \psi$, with $\psi = \nabla \bar{\psi}/(\bar{R}_l \bar{B})$ being the unit vector in the $\nabla \bar{\psi}$-direction.

3.1. Flows

First we study the radial and poloidal structure of the particle flows. As we will see, the flows in global simulations exhibit...
qualitatively different features from the local results. In local theory the flows should be divergence-free on each flux surface in isolation. This is broken in the global case where radial flows play an important role in making the total flow divergence-free. Before discussing the flows in the fixed $\Phi$ and fixed $n_e$ similarity classes, we express the toroidal and poloidal flows, $V_T$ and $V_p$, in terms of $g$,

$$V_T = \frac{B_p}{nB} \int d^3v v g + \frac{T}{mB^2} \int d^3v \left[ \frac{p'}{p} + \frac{Ze\Phi'}{T} \right] + \frac{IB_p}{nB^2} \Phi' \int d^3v + \frac{IB_p}{2nB \partial \psi} \int d^3v^2 g, \quad (15)$$

$$V_p = \frac{B_i}{nB} \int d^3v v g - \frac{T}{mB} \int d^3v \left[ \frac{p'}{p} + \frac{Ze\Phi'}{T} \right] - \frac{B_i^2}{nB} \Phi' \int d^3v - \frac{B_i^2}{2nB \partial \psi} \int d^3v^2 g, \quad (16)$$

where a prime denotes a $\psi$ derivative and $\rho = nT$. The above expressions are accurate to first order in $\delta B_i/B$, and thus include corrections due to the gyrophase dependent part of the distribution function $f \approx -\rho \cdot \nabla f$, where $\rho = \Omega \times b \times \psi$ is the gyroradius vector. In the global theory, $f$ contributes with a $-\rho \cdot \nabla g$ term, which gives the additional corrections to the diamagnetic and $E \times B$ flows on the second rows of the above equations. Equation (15) was calculated in [16] (note that $g$ in [16] is defined differently), and (16) is calculated analogously. We note, that while all terms are comparable in (15), the global corrections to $V_T$ are small in $B_p/B$ compared to the usual expression (the first line of (16)); nevertheless, we keep them for completeness.

Since all the terms in $V_p$ are proportional to $B_p/B$, we factor out this trivial poloidal dependence and define the poloidal flow coefficient

$$k_p = \frac{Ze \langle B^2 \rangle}{IB_p} \left( \frac{d^3v}{d\psi} \right)^{-1} V_p, \quad (17)$$

which reduces to the conventional flux function parallel flow coefficient in the local limit [16] (assuming the lowest order distribution to be a flux function).

### 3.1.1. Fixed $\Phi$ profile flows.

Using (15)–(17) and the fixed $\Phi$ input profiles in figure 1, we obtain the ion flows, $k_p$ and $V_p$, displayed in figure 2.

For the toroidal flows—even though the terms in the second line of (16) are negligible—global effects have an impact through the modifications to $g$. Comparing the global toroidal flow results, figures 2(a), (b), (e) and (f), to the corresponding local ones, figures 2(c), (d), (g) and (h), the most striking difference is that close to the LCFS the toroidal flow changes sign at the high-field side (HFS, $\theta = \pi$). As a general trend seen at all poloidal locations the global toroidal flows are elevated in the core plasma, and reduced in the pedestal.

The poloidal flow coefficients are flux functions in the local case, as seen in figures 2(k), (l), (o) and (p). However, the corresponding global results exhibit complex radial–poloidal features, shown in figures 2(i), (j), (m) and (n). In particular, significant poloidal variations appear in the flows, that include sign changes.

The high field side (HFS, $\theta = \pi$, thick lines) and low field side (LFS, $\theta = 0$, thin lines) toroidal and poloidal flows are shown in figures 3(a)–(c) and (d)–(l), respectively. The electron flows are mostly local due to their small orbit width and our low flow ordering. However, for ions, changing from
local (dashed lines) to global (solid lines) simulations leads to important changes. For instance, in the global case, while the LFS toroidal flows monotonically increase for both ion species throughout radial range plotted, their HFS counterparts decrease in the pedestal, and even change sign for deuterium. On the other hand, for a given ion species, the effects of changing its role from bulk to impurity are rather small, and they are similar in the global and local simulations.

Comparing the differences between the bulk D (blue curves: D bulk; red: He bulk). In the weakly collisional limit of the local theory, even those flow contributions, which are ultimately caused by collisions, become independent of collision frequency. The observed weak variation with changing ion concentration seen here is the result of these cases not being asymptotically collisionless and due to interspecies coupling (as confirmed by simulations with artificially increased collisionality, not shown here). This feature remains valid in the global case as well.

3.1.2. Fixed $n_e$ profile flows. In contrast to the fixed $\Phi$ scenario, in the fixed $n_e$ scenario both $\Phi$ and the ion density profiles change with ion composition, which is expected to be reflected in the ion flows. Since these profile changes are limited to the pedestal region, this is where corresponding effects are expected in the local theory. All modifications to local flows outside the pedestal are the result of changes in collisionality, and thus should be similar in the two similarity classes. In the global theory the effect of the changes in the pedestal profiles will propagate outside the pedestal due to the radial coupling of $g$. It is important that, although in the pedestal $\Phi$ and the ion density gradients change in the scan, the $\eta$ gradient is not changed due to the construction of our model profiles. This means that any differences observed are not due to changes in $\partial_{\psi} f_M$, but due to changes in the finite orbit width effects (the magnitude of the radial electric field is reduced with increasing He concentration).

The flows depicted in figures 4 and 5 do not reveal a striking variation with plasma composition. If we compare the LFS ion flows in the pedestal (thin lines, sub-figures: (a) and (b), (d) and (e); at $\psi = 0$) in figure 4 to the corresponding fixed $\Phi$ figure, figure 3, we indeed see a stronger effect of exchanging bulk and impurity species, although the two different scans produce curves with the same qualitative features. On the other hand, the HFS flows are not affected as strongly. Overall, the effect of changing the helium concentration is small in both scans. Thus, for our low collisionality, slight variations in density profiles do not matter much. The similarities between the two scans can also be verified by looking at the full poloidal dependence of the flows, shown in figure 5 for the bulk helium simulation.

Since we have established that the electron dynamics is not too much affected by our low-flow ordered ions, and the $n_e$ profile is held fixed, we expect the poloidal electron dynamics to exhibit only a modest change in the scan. Comparing the differences between the bulk D (blue) and bulk He (red) curves in between figures 4(f) and 3(f), we find that this is indeed the case. On the other hand, the toroidal flow of electrons changes in the fixed $n_e$ scan, as the radial electric field varies with ion composition.

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**Figure 3.** Toroidal (a)–(c) and poloidal (d)–(f) flows at the LFS ($\theta = 0$, thin lines) and HFS (thick, $\theta = \pi$), in the fixed $\Phi$ scan. Main species is deuterium (blue lines) or helium (red). Solid (dashed) lines correspond to global (local) results.

**Figure 4.** Toroidal (a)–(c) and poloidal (d)–(f) flows at the LFS ($\theta = 0$, thin lines) and HFS (thick, $\theta = \pi$), in the fixed $n_e$ scan. Main species is deuterium (blue lines) or helium (red). Solid (dashed) lines correspond to global (local) results.
3.1.3. Interplay of the poloidal and radial dynamics. In the global simulations we found that the poloidal flow can change sign between different poloidal locations. This is possible because the divergence of the radial flux can make the total radial-poloidal fluxes divergence free. (We use the term ‘flux’ instead of ‘flow’, because the radial variation of the density is not negligible in our simulations.) It is therefore instructive to consider the full radial–poloidal structure of the fluxes. Figure 6 shows a stream plot of the fluxes in the poloidal and radial directions overlaid on top of the poloidal flows, for the same case as shown in figures 2(i)–(d). To account for the vastly different length-scales in the $\nabla \theta$ and $\nabla \psi$ direction, the fluxes are normalized to typical pedestal and poloidal lengths, specifically $(\Gamma / \psi/(\Delta r), \Gamma / \theta/(2\pi a))$, where $\Delta r$ is the pedestal width in meters, $a$ the minor radius on the outboard side and $\theta$ and $\psi$ are unit vectors in the $\nabla \theta$ and $\nabla \psi$ direction, respectively.

As seen in the lower panels of figure 6, the dynamics of the local simulations is rather simple: the small radial fluxes are superimposed on weakly varying poloidal fluxes. In contrast, in the global simulations we find a much richer pattern of fluxes, with stagnation points and vortices in the radial–poloidal plane. Sufficiently far from the pedestal the flows approach their local behavior. The more complex radial flow patterns are not completely localized to the pedestal, but extend a few orbit widths into the core region, which is more visible for the deuterium species.

The vortices in figure 6 depend on the values of radial and poloidal fluxes, and are thus sensitive to the slight shifts in flows observed by changing plasma composition. To only consider the spatial variations of the fluxes, we evaluate the vorticity, defined as

$$\omega = \frac{1}{\hat{r}} \hat{\varphi} \cdot \nabla \times \Gamma \approx \frac{1}{\hat{r}} \left( \frac{\partial G}{\partial r} - \frac{\partial G}{\partial \theta} \right).$$

The vorticities corresponding to figure 2 are displayed in figure 7. Just like the flows, the vorticities are largely unaffected by exchanging bulk and impurity species, and both helium and deuterium display similar structures. In particular, both species display ‘V’-like arms of high vorticity in the pedestal. The apparent differences between the He and D flows in figure 2 may be due to constant flows that mask the radial and poloidal variations, which are more sensitive to global physics. Similarly, sloped vorticity structures extend from the pedestal into the core, and reveal global effects reaching far into the core. It is interesting to note that the slope of the arms is different between the different species, so that the helion vorticity structure extends over all poloidal angles within the width of the pedestal. This behavior is
consistent with helium flows approaching their local values sooner due to their smaller orbit width.

The divergence of the radial fluxes is strongly affected by a radial variation in the diamagnetic flux, and thus it is expected that radially global flow effects are localized to regions where the density or the driving gradients abruptly change. For our model profiles, the density drops inside the pedestal, and the ion temperature gradient rapidly increases at the pedestal top (as expected in a real pedestal). In order to demonstrate the effect of the location of changes in diamagnetic flow strength, we modify our ion temperature profiles. In a scan, we increase the radial length scale over which the logarithmic temperature gradient transition from its core value to its pedestal value; see the corresponding temperature profiles and logarithmic gradients in figure 8 (transition length scale increases from violet to yellow).

Increasing the transition region has a twofold effect: the transition becomes less abrupt, and the effective location where the transition happens moves further outside the pedestal. As a result, the radially global effects in the flow structure become weaker and start to extend further away from the pedestal, as illustrated in figure 9. We also consider a temperature profile with no transition region (red curve) in figures 8, and 9(g) and (h). This shows much weaker, but still visible, deviations from the local simulation in terms of flow patterns. However we have to interpret the ‘no-transition’ results carefully, since in this case the sources were non-negligible even close to the radial boundaries. Nevertheless, it also underlines the importance of the changes in the ion temperature gradient in driving unexpected poloidal flow patterns.

Finally, we consider the poloidal structure of the poloidal flows in the middle of our pedestal region for the various temperature profiles of figure 8. The poloidal flow coefficients at $\psi^c = -0.563$ are shown in figure 10 with the same color coding. For the baseline case (violet line) there are substantial poloidal variations of $k_p$ for both ion species, being higher (or more positive) on the HFS, and lower (more negative) on the LFS. The variation is not sinusoidal, and the local maxima and minima (several of them) appear at poloidal locations away from the mid-plane. With increasing transition length (cyan and yellow curves), the poloidal variation becomes milder, while the minima move to the outboard mid-plane and merge, and the maxima move towards the upper and lower parts of the flux surface. In the no-transition case (red curve), the poloidal variation is weak, but still present, and the global value of $k_p$ is lower than the local one. For electrons (figure 10(c)), the poloidal flows essentially remain local (note the magnified y-axis scale).

### 3.2. Fixed $\Phi$ radial flows and fluxes

To get a clearer picture of the effects of helium concentration on transport, we calculate the total radial particle, conductive heat and toroidal momentum fluxes in the fixed $\Phi$ scan. These are displayed in figure 11, normalized by the core species...
density $\hat{n}_0$ to assist the comparison of the trace and non-trace scenarios.

From figure 11, we can make a few general observations. Firstly, the electron fluxes are practically local by virtue of their small orbit width and large flows, so the electron global and local curves almost overlap (except for the momentum flux figure 11(i), which has no physical relevance as it is small in the electron-to-ion mass ratio—we show it nevertheless for completeness). Since electrons are often omitted from neo-classical simulations, it deserves mention that they can develop a substantial particle flux inside the pedestal. This is the result of the large electron temperature gradient, and it is also present in local simulations.

Secondly, as seen in figures 11(a), (b), (d) and (e), the global ion fluxes in the near-pedestal core tend to be reduced compared to the corresponding local fluxes. Modifications to the ion heat flux compared to the conventional local theory have been predicted by analytical models [32–35] retaining the $v_i \cdot \nabla g$ term, however in our simulations the radial coupling from the $v_m \cdot \nabla g$ also plays an important role in setting the radial fluxes. Here, the modifications are especially notable for the particle fluxes figures 11(a) and (b), which change sign compared to the local results in the near-pedestal core. The width of the affected region scales with the orbit width and is thus larger for D than He; accordingly, the fluxes reach local values further away from the pedestal in the D plasma. Such ‘overshoot’ behavior is also seen in the momentum fluxes figures 11(g) and (h), which instead are increased in the near-pedestal core compared to their local value (that is zero).

The flux surface average species-summed toroidal angular momentum balance states that the named quantity changes in time due to a divergence of the radial momentum transport ($\partial_t(\sum_z \hat{n}_z \hat{\Omega}_z)$), a torque corresponding to any radial currents ($\sum_z \sum_m Z_m \hat{I}_z$), or momentum sources. In our steady state simulations these three contributions should add up to zero. However, in the calculations presented here there are no momentum sources, thus any momentum transport requires the existence of a radial current. This is indeed the case: figures 12(a) and (c) show the corresponding finite radial currents and toroidal angular momentum transport, respectively. (Recall that we do not enforce the ambipolarity of fluxes, and the radial electric field is not solved for in our simulations—but is an input—while the flows are outputs.) This explains why the particle fluxes are below the local values on one side of the pedestal, and above on the other side: the current must integrate to zero over the entire domain for the momentum transport to approach its local value (i.e. vanish) far from the pedestal. We note that although there are non-intrinsically ambipolar processes in the pedestal which could balance our radial currents (due to orbit losses, ripple fields, etc), the radial current we observe is not a necessary feature, but rather a consequence of not allowing for momentum sources. In appendix C we demonstrate that radial currents can be replaced by momentum sources, and it does not have a significant effect on the flow structures.

From figure 12(c), we see that the total momentum flux has roughly the same peak value in both D and He plasmas, although the shape of the curve is wider in the bulk deuterium simulation, again due to the larger orbit width. We emphasize that the finite momentum transport observed here is purely a

![Figure 11. Particle (a)–(c), heat (d)–(f) and momentum (g)–(i) fluxes for bulk D (blue curves) and He (red) plasmas in the fixed $\Phi$ scan. Solid (dashed) lines are global (local) results.](image-url)
make the helium density pedestal sharper than the deuterium density pedestal, which results in a lower $n_{\text{He}}$ further out in the pedestal, and thus a reduced heat flux, from $\vec{q} \propto \vec{n}^2$. Since the ion heat fluxes in the global simulations peak further out compared to the local simulations (figures 11(d) and (e)), the global peak values of $\vec{q}$ are also affected by the reduced $n_{\text{He}}$ in the buffer region, which may be a contributing factor to the reduction of the global $q_{\text{He}}$ compared to the local value.

4. Conclusions

We have studied finite orbit width effects on the neoclassical toroidal and poloidal flows and cross field fluxes, in density pedestals of deuterium–helium mixture plasmas. In a radially global treatment we allow for ion orbit width scale radial density variations and strong radial electric fields, as long as the ions are electrostatically confined and are characterized by subsonic flow speeds. The deuterium–helium ratio scans were performed keeping either the electrostatic potential variation or the electron density profile fixed, leading to surprisingly similar results.

The perturbed neoclassical distribution is modified compared to the radially local treatment, since magnetic and $E \times B$ drift contributions to the advection of the perturbed distribution need to be retained. In addition, non-standard terms appear in the expressions for the flows, corresponding to an $E \times B$ advection of poloidal density perturbations and, more importantly, to the radial variation of diamagnetic fluxes. The resulting poloidal flows exhibit complex radial–poloidal features which vary on a small radial scale, including poloidal sign changes of the poloidal flow. The main reason is that the poloidally local radial particle fluxes are not divergence free in isolation due to the sharp profile variations, which require poloidal return flows to make the total fluxes divergence free. Such flow structures are found to be sensitive to abrupt radial variations in the ion temperature gradient, and can extend quite far into the core if the ion temperature gradient transitions between its core and pedestal value on a long radial scale.

The near-pedestal core values of the global neoclassical particle and conductive ion heat fluxes are often reduced compared to the local results, as a result of an overshoot of decreased fluxes away from the pedestal. Inside the pedestal the heat fluxes are mostly reduced compared to their local values.

We observe a finite radial current, which at least partially arises as no momentum sources were included in these simulations. However it can also represent a physically meaningful charge separation process due to finite orbit width effects, which in steady state needs to be compensated by other non-intrinsically ambipolar processes. The effects of replacing radial current with momentum sources is the subject of ongoing investigation.

The sizable neoclassical toroidal angular momentum transport we observe only appears in global theory. The momentum flux, when normalized to represent an effective Prandtl number, takes on values (few tens of percent)
comparable to experimental values of the effective Prandtl number observed in the plasma core. This is a potentially important observation since the heat fluxes in the pedestal can be dominated by the neoclassical ion heat flux. This implies that if our results extraplate to large ion temperature gradients (where a full-f treatment is unavoidable), radially global effects might account for a significant fraction of the momentum transport in the inner region of the pedestal.

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Appendix A. Model pedestal profiles and magnetic geometry

Due to the constraints on the T and \( \eta \) profiles (7), we use simple model profiles for our simulations. Specifically, an \( \text{mtanh} \) transition between two constant gradient regions is implemented as

\[
X = \frac{X_{\text{ped}} + X_{\text{SOL}} + (a - b) w_{\text{ped}}/2}{2} - \frac{X_{\text{ped}} - X_{\text{SOL}} + (a + b) w_{\text{ped}}/2}{2} \tanh (r) + \frac{a(\psi - \psi_0)e^{-\tau} + b(\psi - \psi_0)e^{\tau}}{e^{-\tau} + e^{\tau}},
\]

where \( X \) is a generic profile, \( r = (\psi - \psi_0) w_{\text{ped}}/2 \), \( w_{\text{ped}} \) is the pedestal width, \( a \) (\( b \)) the core (SOL) asymptotic profile gradients; \( \psi_0 \) is the position of the middle of the pedestal. Here ‘SOL’ represents the numerical buffer region outside \( \psi = 0 \).

The magnetic field is assumed not to vary notably over the pedestal region, and we thus use a radially constant, local Miller geometry [30] with parameters: \( \kappa = 1.58 \), \( s_x \equiv (r/\kappa)dx/dr = 0.479 \), \( \partial R/\partial r = -0.14 \), \( \delta = 0.24 \), \( s_y \equiv (r/\sqrt{1 - \delta^2})d\delta/dr = 0.845 \), \( q = 3.5 \), \( \epsilon \equiv r/R = 0.263 \), where \( \kappa \) is the elongation, \( \delta \) the triangularity and the corresponding \( s_x \) parameters measure their shear.

Appendix B. Insensitivity to boundary conditions

Based on the size of the global term in the DKE (8)—which sets the radial coupling—the radial correlations are expected to decrease outside the pedestal region. As a consequence, the flows and fluxes in the pedestal are essentially decorrelated from the boundary conditions, provided that the boundaries are sufficiently far away from the pedestal.

To demonstrate this, we performed identical simulations with Neumann boundary conditions (\( \mathbf{n}_0 \cdot \nabla \mathbf{g} = 0 \)) instead of Dirichlet (\( \mathbf{g} = \mathbf{g}_{\text{local}} \)). The resulting poloidal flows are displayed in thin lines figure 15 and largely overlap around the pedestal with the Dirichlet results indicated with thick lines—even though the Dirichlet boundary condition can introduce massive oscillations near the boundaries.

The poloidal flows were chosen for this test as they are particularly sensitive to numerical errors, since their evaluation involves a derivative of simulation outputs (the final term in (15)). Similar or higher degrees of agreement are also found for the poloidal variation of \( V_{\phi} \) in the middle of the pedestal, and other quantities such as the radial fluxes and sources. Thus, we concluded that the results indeed are largely independent of the boundary conditions.

Appendix C. Radial current replaced by momentum sources

We observe a finite radial current in our simulations, which is balanced by non-quasineutral particle sources. If this would be the only radial current, the corresponding time evolution of the electric field would be inconsistent with the assumption of steady state. Even though it cannot be ruled out that other, not modeled, non-intrinsically ambipolar processes cancel our radial current, the appearance of a radial current in the simulation may nevertheless be concerning. Note however, that since we do not solve for the radial electric field our current is not a source of any numerical inconsistency in the simulation.

The torque from the radial current appears in the species-summed toroidal angular momentum equation, and in steady state it is balanced by the divergence of the toroidal angular momentum flux, and momentum sources, if any. In the simulations presented here no momentum sources were considered, therefore it is possible that the current we observe develops merely to balance the radial variation of the
momentum flux, and that a radial current may not be necessary if we allow for momentum sources. Here we show results indicating that this is the case, although a thorough investigation of the problem is outside the scope of this paper.

Momentum sources can arise from numerous effects, a few candidates near the edge are: the radial variation of turbulent momentum fluxes, atomic physics processes [41], or orbit loss effects [42]. However, we will not dwell on the physical origin of the momentum sources, but instead solve for the radial dependence of a momentum source profile by requiring the radial current to vanish, $\sum_a Z_a \hat{f}_a = 0$. This requirement represents only one additional constraint per radial grid point (in contrast to one for each species), and accordingly, it allows us to solve for only one new radial profile. To eliminate the corresponding degrees of freedom we assumed momentum sources for the various species to be proportional to the mass and the concentration of the species in the core, $\hat{S}_{nm} \propto m_n r_{lim} \hat{S}_m$, and we solve only for $\hat{S}_m$. The velocity space structure of the momentum sources was taken so that they do not contribute to parallel heat fluxes, and we assume the sources to be poloidally uniform. These choices are not motivated by any particular physical process, but should be sufficient for our purposes.

Using the baseline deuterium bulk plasma case, we performed a simulation where we allowed for momentum sources by the scheme specified above. In figure 16 we show particle and momentum sources for the simulation with zero radial current (red curves) and compare it to the results without momentum sources (blue curves). As clearly seen in figure 16(e), it is possible to enforce a vanishing radial current (red curve is zero), but in that case there is a need for finite momentum sources (see red curve in figure 16(d)). The particle sources, shown in figures 16(a)–(c), have changed to achieve a zero net charge source. They still share qualitative similarities with those in the simulation without momentum sources: in both cases the particle sources have a positive peak a little inside the pedestal top and drop towards the separatrix in such a way that they change sign around the middle of the model pedestal.

Importantly, the interaction of the radial and poloidal fluxes and the corresponding complex flow patterns are not very sensitive to the replacement of radial currents with momentum sources in the simulation. This is perhaps best illustrated by comparing vorticities, see figure 17, where (a) and (b) shows results with zero radial current, and the case without momentum sources is shown in (c) and (d).

While the issue deserves a more detailed study, here we have demonstrated that radial currents are not a necessary feature of our simulations, and that from the point of view of flows it is of secondary importance whether the radial variation of the toroidal angular momentum is balanced by a torque from a radial current or by momentum sources. The red curve of figure 16(d) and the blue curve of (e) are proportional to the radial variation of the total toroidal angular momentum flux in their respective cases ($\hat{S}_{nm}$ is here defined to make the proportionality constant the same in both cases). Their similarity suggests that the momentum fluxes are similar in the two cases. Without adding a corresponding figure we note that this is indeed the case, although the magnitude of the momentum transport is somewhat higher in the zero radial current case, as expected from comparing the magnitudes in figures 16(d) and (e).

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