

Poloidal impurity asymmetries, flow and neoclassical transport in pedestals in the plateau and banana regimes

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Charge exchange recombination spectroscopy (CXRS) measures the radial electric field in the pedestal by measuring the impurity density, temperature and flow. Combined outboard and inboard CXRS measurements allow poloidal variations that arise due to the poloidal variation of the magnetic field to be determined. At present, impurity neoclassical pedestal models avoid the complications of treating finite poloidal gyroradius effects by assuming the impurity charge number is large compared with the main ion charge number. These models are extended slightly by retaining the impurity radial pressure gradient to demonstrate that no substantial effect occurs due to impurity diamagnetic effects. More importantly, the neoclassical model is significantly extended to obtain a more comprehensive treatment of the main ions in the plateau and banana regimes. A parallel impurity momentum equation is derived that is consistent with previous results in the banana regime and reduces to the proper large aspect ratio form required in the plateau regime. The implications for interpreting the CXRS measurements are discussed by writing all results in terms of the gradient drive and poloidal flow.

Key words: fusion plasma, plasma confinement, plasma flows

1. Introduction

The pedestal region just inside the last closed flux surface on a tokamak is characterized by strong radial gradients in pressure and electrostatic potential in both high or H mode (Wagner *et al.* 1982) and improved or I mode (Whyte *et al.* 2010) confinement regimes. Both regimes tend to have similar ion temperature profiles, but H mode has much stronger density gradients than I mode. Charge exchange recombination spectroscopy (CXRS) diagnostics of impurities has enabled the measurement of the strong radial electric field in the pedestal (McDermott *et al.* 2009; Viezzer *et al.* 2013a) as well as in-out asymmetries in this field and in the impurity density (Churchill *et al.* 2013, 2015; Viezzer *et al.* 2013b; Theiler *et al.* 2014). The scale lengths of the radial electric field can be as small as a poloidal ion gyroradius, making conventional neoclassical treatments (Hinton & Hazeltine 1976) inappropriate (Trinczek *et al.* 2023). To cope with the limitations of the conventional neoclassical orderings, but maintain a local treatment of transport, Helander (1998) employed a high charge number ordering of the impurities that allows some of

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the behaviour of the impurities to be understood for banana regime background ions. In particular, he demonstrated that large background or main ion gradients poloidally redistribute impurity ions to reduce both their parallel friction with the main ions and the neoclassical particle flux, and may do so by impurity accumulation on the high field side of a tokamak. Subsequent work considered strong rotation (Fülöp & Helander 1999) and plateau regime background ions Landreman, Fülöp & Guszejnov (2011). For banana and plateau regime main ions the leading modification to the Maxwellian is from a poloidal gyroradius over a radial scale length correction. Alternately, for the collisional Pfirsch–Schlüter background ions considered by Fülöp & Helander (2001) and Maget *et al.* (2020*a,b*) the leading modification is a mean free path over parallel connection length correction. In addition, because CXRS measures the impurity flow to determine the radial electric field, the banana regime formulation of Helander has been recast into a form that employs the measured poloidal impurity flow in place of a term that requires solving the complicated kinetic equation for the main ion species in the presence of impurities (Espinosa & Catto 2017*a,b*, 2018). In all these models the poloidal variation of the magnetic field is responsible for the poloidal variation of the impurity density, which is then responsible for the poloidal variation of the electric field.

As the pedestal may be in either the plateau or banana regime, the purpose of the material to follow is to build on these earlier treatments by demonstrating that these regimes share many of the same characteristics. In particular, the poloidal variation of the impurity density in the plateau regime and the large aspect ratio limit of the banana regime are shown to be the same. Moreover, the treatment here allows the retention of the impurity pressure gradient term neglected as small in these earlier treatments. This minor generalization is accomplished by allowing moderate impurity charge numbers such as nitrogen, carbon, and boron, and using an aspect ratio expansion for the impurity pressure gradient terms, and means that impurity flows need no longer be on a flux surface. All other terms are treated with the same generality as earlier treatments. In addition, the treatment here improves the earlier plateau regime solution of the main ion kinetic equation and its treatment of ambipolarity.

The next section introduces the tokamak notation and coordinates employed. Section 3 focuses on the general expressions for the parallel impurity momentum equation, quasineutrality, the radial impurity flux and the impurity flow, all with the slightly improved treatment of the impurity pressure. The general expressions are specialized to banana regime main ions in § 4 to show the results are consistent with earlier treatments when impurity pressure gradient terms are ignored. Plateau regime main ions are considered in § 5 in more detail as the treatment here generalizes the earlier treatment of Landreman *et al.* (2011). Section 6 presents approximate solutions for poloidal variation of the impurity density variation in the plateau and banana regimes as well as detailed discussion of radial particle transport. The implications for the diffusion and convection form of the impurity continuity equation are noted in § 7. A summary of the results is given in § 8, as well as a table of model predictions.

2. Tokamak geometry and notation

The magnetic field of an axisymmetric tokamak can be written as

$$\mathbf{B} = I\nabla\zeta + \nabla\zeta \times \nabla\psi = \nabla(\zeta - q\vartheta) \times \nabla\psi = B\mathbf{b}, \quad (2.1)$$

where ψ is the poloidal flux function, ζ is the toroidal angle (with $|\nabla\zeta| = R^{-1}$), ϑ is the poloidal angle, q is the safety factor, \mathbf{b} is a unit vector along \mathbf{B} and $I = I(\psi) = RB_r$ with

R the major radius and B_t the toroidal magnetic field. By picking ϑ such that

$$\mathbf{B} \cdot \nabla \vartheta = |I|/qR^2 = q^{-1}|\mathbf{B} \cdot \nabla \zeta|, \tag{2.2}$$

q will be a flux function $q = q(\psi)$. Other useful relations are $\mathbf{B} \times \nabla \psi = I\mathbf{B} - B^2 R^2 \nabla \zeta$, $|\nabla \psi| = RB_p$, $\nabla \zeta \cdot \nabla \psi = 0 = \nabla \zeta \cdot \nabla \vartheta$ and $\nabla \psi \times \nabla \vartheta \cdot \nabla \zeta = \mathbf{B} \cdot \nabla \vartheta$, with B_p the poloidal magnetic field. The toroidal current is taken to be in the $\nabla \zeta$ direction to make $B_p > 0$ and $\mathbf{B} \cdot \nabla \vartheta > 0$, and the low field side (LFS) equatorial plane is always taken to be $\vartheta = 0$ with ϑ increasing in the $\mathbf{B}_p = \nabla \zeta \times \nabla \psi$ direction. The toroidal magnetic field can be in the co-current ($B_t > 0$) or counter-current ($B_t < 0$) direction. Alcator C-Mod viewed from above normally has $\nabla \zeta$ in the clockwise direction with $B_t > 0$ (McDermott *et al.* 2009; Theiler *et al.* 2014), while ASDEX Upgrade (AUG) viewed from above typically has $\nabla \zeta$ in the counter-clockwise direction with $B_t < 0$ (Viezzler *et al.* 2013a). Consequently, for standard operation the poloidal magnetic field at the equatorial plane on the LFS points upward in C-Mod and downward in AUG.

In ψ, ϑ, ζ variables the components of any vector \mathbf{A} can be written as

$$\begin{aligned} \mathbf{A} = & (\nabla \psi \times \nabla \vartheta \cdot \nabla \zeta)^{-1} [(\mathbf{A} \cdot \nabla \psi)(\nabla \vartheta \times \nabla \zeta) \\ & + (\mathbf{A} \cdot \nabla \vartheta)(\nabla \zeta \times \nabla \psi) + (\mathbf{A} \cdot \nabla \zeta)(\nabla \psi \times \nabla \vartheta)]. \end{aligned} \tag{2.3}$$

In this form it is easy to form the divergence

$$\nabla \cdot \mathbf{A} = \left[\frac{\partial}{\partial \psi} \left(\frac{\mathbf{A} \cdot \nabla \psi}{\mathbf{B} \cdot \nabla \vartheta} \right) + \frac{\partial}{\partial \vartheta} \left(\frac{\mathbf{A} \cdot \nabla \vartheta}{\mathbf{B} \cdot \nabla \vartheta} \right) \right] \mathbf{B} \cdot \nabla \vartheta. \tag{2.4}$$

In a tokamak the flux surface average of a scalar quantity A is defined as

$$\langle A \rangle = (1/V') \oint d\vartheta A / \mathbf{B} \cdot \nabla \vartheta, \tag{2.5}$$

with $V' = \oint d\vartheta / \mathbf{B} \cdot \nabla \vartheta$ and the ϑ integral over a full 2π when $A = A(\psi, \vartheta)$. The flux surface average operating on the divergence of a vector \mathbf{A} gives

$$\langle \nabla \cdot \mathbf{A} \rangle = \frac{1}{V'} \frac{\partial}{\partial \psi} (V' \langle \mathbf{A} \cdot \nabla \psi \rangle). \tag{2.6}$$

Then, for the current density \mathbf{J} , for example, $\langle \nabla \cdot \mathbf{J} \rangle = 0$ will give the ambipolarity condition $\langle \mathbf{J} \cdot \nabla \psi \rangle = 0$ upon integration from the magnetic axis, where the radial current vanishes.

3. Conservation of impurity momentum and number, and quasineutrality

The lowest order momentum conservation equation for the impurities (subscript z , with Z_z charge number and M_z mass, where e is the proton charge and c the light speed) is

$$Z_z e n_z (\nabla \Phi - c^{-1} \mathbf{V}_z \times \mathbf{B}) + \nabla p_z = b F_{zi}^{\parallel} = b M_z \int d^3 v v_{\parallel} C_{zi}, \tag{3.1}$$

where for the low flow speeds considered here the inertial term is negligible. Here, F_{zi}^{\parallel} is the parallel collisional friction between impurities and ions (subscript i), C_{zi} is the collision operator for impurities colliding with the main or background ions, n_z and $p_z = n_z T_i(\psi)$ are the impurity density and pressure, \mathbf{V}_z is the impurity velocity and Φ is the electrostatic

potential. Equilibration with the ions is assumed to give $T_z = T_i$, the ion temperature. Only subsonic rotation is considered. The sonic case was considered by Fülöp & Helander (1999).

To formulate theoretical descriptions that allow all the terms in (3.1) to be the same order for the moderate $Z_z \gg Z_i$ under consideration (with $Z_z n_z \ll Z_i n_i$), the ordering

$$Z_z e \Phi \sim T_i \gg Z_i e \Phi, \quad (3.2)$$

must be assumed to allow $Z_z e n_z \nabla \Phi \sim \nabla p_z$, where Z_i and n_i are the main ion charge number and density. This ordering is not as general as a true pedestal ordering that requires $Z_i e \Phi \sim T_i$ to permit $Z_i e n_i \partial \Phi / \partial \psi \sim \partial p_i / \partial \psi$ (Trinczek *et al.* 2023), but does allow insight into the CXRS measurements. Therefore, the theoretical models developed here all assume

$$\partial p_i / \partial \psi \gg Z_i e n_i \partial \Phi / \partial \psi \gg Z_z e n_z \partial \Phi / \partial \psi \sim \partial p_z / \partial \psi. \quad (3.3)$$

An expression for the radial electric field (E_r) is found by dotting momentum balance by $\nabla \vartheta \times \nabla \zeta$ and neglecting the friction contribution as small to find

$$\begin{aligned} E_r &= -RB_p \frac{\partial \Phi}{\partial \psi} \approx \frac{RB_p}{Z_z e n_z} \frac{\partial p_z}{\partial \psi} + \frac{RB_p}{c} V_z \cdot \nabla \zeta - \frac{IB_p}{cR} \frac{V_z \cdot \nabla \vartheta}{\mathbf{B} \cdot \nabla \vartheta} \\ &\approx \frac{RB_p}{Z_z e n_z} \frac{\partial p_z}{\partial \psi} + \frac{1}{c} (V_i B_p - V_p B_i). \end{aligned} \quad (3.4)$$

Injecting an impurity or using an intrinsic one and ignoring the parallel friction as small, the radial electric field is deduced by measuring the diamagnetic, toroidal flow and poloidal flow contributions, respectively (McDermott *et al.* 2009; Viezzer *et al.* 2013a; Theiler *et al.* 2014; Cruz-Zabala *et al.* 2022). The orderings of (3.2) and (3.3) allow all terms in (3.4) to be the same order. The flux surface averaged electrostatic potential, $\langle \Phi \rangle$, is largely determined by the main ions through conservation of toroidal angular momentum. Measuring the radial impurity pressure gradient and poloidal and toroidal flows in (3.4) allows the radial electric field to be determined. The poloidal variation of the electrostatic potential, $\Phi - \langle \Phi \rangle$, can be rather strong due to the impurities. The poloidal variation of the impurity density is found from conservation of impurity parallel momentum. Impurities can result in strong poloidal variation in $\Phi - \langle \Phi \rangle$ due to the need to maintain quasineutrality. Any contribution from $\partial(\Phi - \langle \Phi \rangle) / \partial \psi$, causes the radial electric field to vary poloidally.

Momentum balance also yields the perpendicular impurity flow velocity $V_{\perp z}$ giving

$$n_z V_z = n_z V_{\perp z} + n_z V_{\parallel z} \mathbf{b} = cB^{-2} \mathbf{B} \times [n_z \nabla \Phi + (Z_z e)^{-1} \nabla p_z] + B^{-1} n_z V_{\parallel z} \mathbf{B}. \quad (3.5)$$

The impurity flow can also be written as

$$n_z V_z = L_z \mathbf{B} + n_z \omega_z R^2 \nabla \zeta - \Upsilon \nabla \vartheta \times \nabla \zeta, \quad (3.6)$$

where the Υ term allows a radial flow departure from a flux surface

$$n_z V_z \cdot \nabla \psi = -\Upsilon \mathbf{B} \cdot \nabla \vartheta = -\frac{cI}{Z_z e B^2} (\mathbf{B} \cdot \nabla p_z + Z_z e n_z \mathbf{B} \cdot \nabla \Phi). \quad (3.7)$$

The angular frequency $\omega_z = \omega_z(\psi, \vartheta)$ contributes to the toroidal flow $V_z \cdot \nabla \zeta = \omega_z + n_z^{-1} L_z \mathbf{B} \cdot \nabla \zeta$. The parallel flow coefficient L_z is related to the poloidal flow and leads to

the useful expression

$$n_z V_z \cdot \nabla \vartheta = L_z \mathbf{B} \cdot \nabla \vartheta = \left[\frac{n_z V_{||z}}{B} + \frac{cI}{Z_z e B^2} \left(\frac{\partial p_z}{\partial \psi} + Z_z e n_z \frac{\partial \Phi}{\partial \psi} \right) \right] \mathbf{B} \cdot \nabla \vartheta. \quad (3.8)$$

In addition, the impurity continuity equation gives

$$0 = \nabla \cdot (n_z V_z) = \mathbf{B} \cdot \nabla \vartheta \left(\frac{\partial L_z}{\partial \vartheta} - \frac{\partial \Upsilon}{\partial \psi} \right). \quad (3.9)$$

The retention of the radial impurity pressure gradient and the poloidal variation of the electrostatic potential and the impurity pressure mean that L_z is not a flux function. In the Helander (1998) treatment $\partial \Upsilon / \partial \psi$ is ignored because Z_z is assumed very large. The poloidal variation of the impurity density and electrostatic potential are responsible for the radial impurity flow that does not occur in standard banana and plateau regime treatments that assume both are flux functions (Hinton & Hazeltine 1976). The small radial flow correction Υ was not considered in earlier treatments that focused on measuring the poloidal variation of the impurity flow on a flux surface (Marr *et al.* 2010; Pütterich *et al.* 2012).

To evaluate the friction in the parallel impurity momentum equation

$$\mathbf{B} \cdot \nabla p_z + Z_z e n_z \mathbf{B} \cdot \nabla \Phi = B F_{zi}^{||} = -B F_{iz}^{||} = -M_i B \int d^3 v v_{||} C_{iz}, \quad (3.10)$$

collisional momentum conservation, $M_z \int d^3 v v_{||} C_{zi} + M_i \int d^3 v v_{||} C_{zi} = 0$, is employed since it is convenient to use the collision operator C_{iz} for the faster background ions colliding with the slower impurities

$$C_{iz} \{f_{i1}\} = \frac{3\sqrt{2\pi} T_i^{3/2} v_{iz}}{4M_i^{3/2}} \nabla_v \cdot \left[\nabla_v \nabla_v v \cdot \nabla_v \left(f_{i1} - \frac{M_i}{T_i} V_{||z} v_{||} f_{i0} \right) \right], \quad (3.11)$$

where $f_i = f_{i0} + f_{i1}$, with f_{i1} the non-adiabatic perturbed ion distribution function and f_{i0} the Maxwellian (which must be a flux function and depend on total energy in the banana and plateau regimes)

$$f_{i0} = n_i (M_i / 2\pi T_i)^{3/2} e^{-M_i v^2 / 2T_i} \approx \langle n_i \rangle [1 - Z_i e (\Phi - \langle \Phi \rangle) / T_i] e^{-M_i v^2 / 2T_i}, \quad (3.12)$$

with $n_i \approx \langle n_i \rangle [1 - Z_i e (\Phi - \langle \Phi \rangle) / T_i]$. It is convenient to keep the perturbed Maxwell-Boltzmann response in f_{i0} . The ion-impurity collision frequency ν_{iz} is defined as

$$\nu_{iz} = 4\sqrt{2\pi} Z_i^2 Z_z^2 e^4 n_z \ell n \Lambda / 3M_i^{1/2} T_i^{3/2}, \quad (3.13)$$

with $\ell n \Lambda$ the Coulomb logarithm, $\nu_{iz} / \nu_{zi} = M_z n_z / 2M_i n_i \ll 1$ and M_i the background ion mass. Evaluating the parallel friction gives

$$F_{iz}^{||} = M_i \int d^3 v v_{||} C_{iz} = M_i n_i \nu_{iz} \left(V_{||z} - \frac{3\sqrt{2\pi} T_i^{3/2}}{2M_i^{3/2} n_i} \int d^3 v \frac{v_{||} f_{i1}}{v^3} \right) = -F_{zi}^{||}. \quad (3.14)$$

Only unlike collisions cause particle transport. The banana regime diffusivity for electrons colliding with the main ions, D_e , is roughly $D_e \sim q^2 \rho_e^2 \nu_{ei} / \varepsilon^{3/2} \propto n_e M_e^{1/2}$, with ρ_e the electron gyroradius, ν_{ei} the electron-ion collision frequency and M_e the electron mass. The

banana regime diffusivity for the faster moving main ions colliding with the slower moving impurities, D_i , is roughly $D_i \sim q^2 \rho_i^2 v_{iz} / \varepsilon^{3/2} \propto Z_z^2 n_z M_i^{1/2}$, with ρ_i the ion gyroradius. Therefore, as long as $Z_z^2 n_z / n_e \gg (M_e / M_i)^{1/2}$ electron transport can be ignored. Then, ambipolarity between the ions and impurities requires

$$Z_i \langle n_i V_i \cdot \nabla \psi \rangle = -Z_z \langle n_z V_z \cdot \nabla \psi \rangle = Z_z \langle \Upsilon \mathbf{B} \cdot \nabla \vartheta \rangle = -(cI/e) \langle F_{iz}^{\parallel} / B \rangle, \tag{3.15}$$

with poloidal variation of Υ (due to n_z and Φ) essential to obtain finite particle fluxes. The poloidal variation of the magnetic field in the parallel friction gives rise to poloidal variation of the potential and the densities. These poloidal density variations must satisfy quasineutrality, which upon taking the poloidal derivative yields

$$\mathbf{B} \cdot \nabla n_e = Z_i \mathbf{B} \cdot \nabla n_i + Z_z \mathbf{B} \cdot \nabla n_z. \tag{3.16}$$

Assuming the temperatures are flux functions, and using a Maxwell–Boltzmann response for the electrons, $n_e \approx \langle n_e \rangle [1 + e(\Phi - \langle \Phi \rangle) / T_e(\psi)]$, and background ions, leads to

$$Z_z \mathbf{B} \cdot \nabla n_z = \langle n_e \rangle \left(\frac{e}{T_e} + \frac{Z_i e}{T_i} \right) \mathbf{B} \cdot \nabla \Phi, \tag{3.17}$$

where the impurity density is assumed small in order not to alter lowest order quasineutrality, $\langle n_e \rangle = Z_i \langle n_i \rangle \gg Z_z \langle n_z \rangle$. Consequently, the potential can be eliminated from the parallel momentum constraint and the solution for n_z must satisfy the solubility constraint $\langle B F_{iz}^{\parallel} \rangle = 0$. Using quasineutrality to rewrite the parallel impurity equation yields

$$\left(1 + \frac{\alpha n_z}{\langle n_z \rangle} \right) \mathbf{B} \cdot \nabla n_z = -\frac{B F_{iz}^{\parallel}}{T_i}, \tag{3.18}$$

where

$$\alpha = Z_z^2 \langle n_z \rangle \tau / Z_i \langle n_e \rangle (1 + \tau), \tag{3.19}$$

is allowed to be order unity or less, and $\tau = Z_i T_e / T_i$. Equation (3.17), as well as (3.4) and the preceding orderings, allow $Z_z e(\Phi - \langle \Phi \rangle) / T_i \sim (n_z - \langle n_z \rangle) / n_z \sim 1$ as well as $Z_z e \langle \Phi \rangle \sim T_i$, but assume $Z_i e(\Phi - \langle \Phi \rangle) / T_i \ll 1$.

The poloidal variation of the impurity density is due to the poloidal variation of the magnetic field in $B F_{iz}^{\parallel}$. Normalizing with $n = n_z / \langle n_z \rangle$ and $b^2 = B^2 / \langle B^2 \rangle$, and introducing $d\theta = \langle \mathbf{B} \cdot \nabla \vartheta \rangle d\vartheta / \mathbf{B} \cdot \nabla \vartheta$ to remove the ϑ dependence of $\mathbf{B} \cdot \nabla \vartheta$, the parallel impurity momentum equation becomes

$$(1 + \alpha n) \frac{\partial n}{\partial \theta} = -\frac{M_i n_i \langle v_{iz} \rangle \langle B^2 \rangle}{\langle n_z \rangle \langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle} b^2 \left(\frac{n_z V_{\parallel z}}{B} - \frac{3\sqrt{2\pi} T_i^{3/2} n_z}{2M_i^{3/2} n_i} \int d^3 v \frac{v_{\parallel} f_{i1}}{Bv^3} \right), \tag{3.20}$$

where $n_i \approx \langle n_i \rangle$ is used in the coefficients on the right side since it gives a negligible correction of order $Z_i e(\Phi - \langle \Phi \rangle) / T_i \sim Z_z (n_z - \langle n_z \rangle) / \langle n_e \rangle \ll 1$. Here, and in the remainder of this and the following sections, $n_i \approx \langle n_i \rangle$ and $p_i \approx \langle p_i \rangle = \langle n_i \rangle T_i$, but $n_z \neq \langle n_z \rangle$.

Taking the poloidal derivative of quasineutrality also allows Υ to be written as

$$\Upsilon = \frac{cIT_i}{Z_z e B^2} \left(1 + \frac{\alpha n_z}{\langle n_z \rangle} \right) \frac{\partial n_z}{\partial \vartheta} = \frac{cI \langle p_z \rangle}{Z_z e B^2} \frac{\partial}{\partial \vartheta} \left[n - 1 + \frac{\alpha}{2} (n^2 - 1) \right]. \tag{3.21}$$

Notice that when Z_z is very large, $\Upsilon \rightarrow 0$ giving $\partial L_z / \partial \vartheta \rightarrow 0$ as in the limit considered by Helander (1998). Interestingly, the lowest order poloidal variation of L_z due to impurity

diamagnetic effects can be retained by assuming the poloidal variation of the magnetic field is weak by ordering

$$\frac{1}{\langle n_z \rangle} \frac{\partial n_z}{\partial \vartheta} \sim \frac{1}{\langle B^2 \rangle} \frac{\partial B^2}{\partial \vartheta} \sim \varepsilon \ll 1. \tag{3.22}$$

This ordering is consistent with the inverse aspect ratio, $\varepsilon = a/R$, expansion necessary in the plateau regime, where a is the minor radius. In the banana regime, this expansion is only necessary to treat impurity pressure terms, but illustrates how their behaviour enters to a limited extent. In the banana regime all other terms can be retained for general B , and therefore, for quite general n_z as long as the poloidal ion gyroradius is small compared with the radial scale lengths. The aspect ratio expansion means

$$\begin{aligned} \frac{1}{b^2} \frac{\partial}{\partial \vartheta} \left[n - 1 + \frac{\alpha}{2}(n^2 - 1) \right] &= \frac{\partial}{\partial \vartheta} \left[\frac{n - 1}{b^2} + \frac{\alpha}{2b^2}(n^2 - 1) \right] \\ &- \left[n - 1 + \frac{\alpha}{2}(n^2 - 1) \right] \frac{\partial}{\partial \vartheta} \left(\frac{1}{b^2} \right), \end{aligned} \tag{3.23}$$

where the last term is order ε^2 . Consequently, impurity diamagnetic modifications of order $Z_i \varepsilon / Z_z$ are retained by writing γ as

$$\gamma = \frac{cI \langle p_z \rangle}{Z_z e \langle B^2 \rangle} \frac{\partial}{\partial \vartheta} \left[\frac{n - 1}{b^2} + \frac{\alpha}{2b^2}(n^2 - 1) \right] + \Delta, \tag{3.24}$$

with $\langle \gamma \mathbf{B} \cdot \nabla \vartheta \rangle = \langle \Delta \mathbf{B} \cdot \nabla \vartheta \rangle$ and $Z_i \varepsilon^2 / Z_z$ corrections from Δ

$$\Delta = \frac{cI \langle p_z \rangle}{Z_z e \langle B^2 \rangle} \left[n - 1 + \frac{\alpha}{2}(n^2 - 1) \right] \frac{\partial}{\partial \vartheta} \left(1 - \frac{1}{b^2} \right). \tag{3.25}$$

Ignoring the Δ term as small in $\nabla \cdot (n_z \mathbf{V}_z) = 0$ and integrating (3.9) leads to

$$\frac{n_z \mathbf{V}_z \cdot \nabla \vartheta}{\mathbf{B} \cdot \nabla \vartheta} = L_z \approx K_z(\psi) + \frac{\partial}{\partial \psi} \left\{ \frac{cI \langle p_z \rangle}{Z_z e \langle B^2 \rangle} \left[\frac{n - 1}{b^2} + \frac{\alpha}{2b^2}(n^2 - 1) \right] \right\}, \tag{3.26}$$

with K_z a flux function associated with the poloidal flow. The preceding and

$$\frac{n_z \mathbf{V}_z \cdot \nabla \vartheta}{\mathbf{B} \cdot \nabla \vartheta} = \frac{n_z V_{||z}}{B} + \frac{cI}{B^2} \left(n_z \frac{\partial \Phi}{\partial \psi} + \frac{1}{Z_z e} \frac{\partial p_z}{\partial \psi} \right), \tag{3.27}$$

allow the parallel impurity flow to be written as

$$\frac{n_z V_{||z}}{B} = K_z(\psi) - \frac{cI}{B^2} \left(n_z \frac{\partial \Phi}{\partial \psi} + \frac{1}{Z_z e} \frac{\partial \langle p_z \rangle}{\partial \psi} \right) + \frac{cI}{Z_z e B^2} \frac{\partial}{\partial \psi} [\alpha \langle p_z \rangle (n - 1)], \tag{3.28}$$

where in $\langle p_z \rangle$ terms the radial variation of B is weak compared with that of n_z , n_i and T_i .

To make further progress more details of the solution f_{i1} are required. The required details can be obtained by considering the background ions to be in the banana ($v_* \equiv v_{ii} qR / v_i \varepsilon^{3/2} < 1$) or plateau ($1 < v_{ii} qR / v_i \varepsilon^{3/2} \equiv v_* < 1 / \varepsilon^{3/2}$) regimes, where $v_{ii} = 4\sqrt{\pi} Z_i^4 e^4 n_i \ell n \Lambda / 3M_i^{1/2} T_i^{3/2}$ is the ion-ion collision frequency, v_* is the ion collisionality and $v_i = (2T_i / M_i)^{1/2}$ is the ion thermal speed. The banana regime is considered next and then the plateau regime. In both cases the impurities may be collisional even

for moderate Z_z/Z_i , as $v_{zz}/v_{ii} = Z_z^4 n_z M_i^{1/2} / Z_i^4 n_i M_z^{1/2} \sim \alpha (Z_z/Z_i)^{3/2}$ gives $v_{zz} qR/v_z \sim \alpha (Z_z/Z_i)^2 (v_{ii} qR/v_i)$, with v_{zz} the impurity–impurity collision frequency and $v_z = \sqrt{2T_i/M_z}$ the impurity thermal speed. The preceding indicates the impurities become collisional when $\alpha (Z_z/Z_i)^2 > 1$. Collisional background ions are not considered here, but were investigated by Fülöp & Helander (2001) and Maget *et al.* (2020a,b).

4. Banana regime background ions

In the banana regime ($v_{ii} qR/v_i < \varepsilon^{3/2}$) the background ion kinetic equation to be solved in total energy, $E = v^2/2 + Z_i e \Phi / M_i$, and magnetic moment, $\mu = v_{\perp}^2 / 2B$, variables is

$$v_{\parallel} \mathbf{b} \cdot \nabla h_1 = C_1 \left\{ h_1 - \frac{I v_{\parallel}}{\Omega_i} \frac{\partial f_{i0}}{\partial \psi} \right\}, \tag{4.1}$$

where C_1 is the ion–ion plus ion–impurity collision operator, $\Omega_i = Z_i e B / M_i c$ is the ion cyclotron frequency,

$$f_{i0} = \eta(\psi) (M_i / 2\pi T_i)^{3/2} e^{-M_i E / T_i} \approx \langle n_i \rangle [1 - Z_i e (\Phi - \langle \Phi \rangle) / T_i] e^{-M_i v^2 / 2T_i}, \tag{4.2}$$

with $n_i = \eta e^{-Z_i e \Phi / T_i} \approx \langle n_i \rangle [1 - Z_i e (\Phi - \langle \Phi \rangle) / T_i]$ as before, with $\eta = \langle n_i \rangle e^{Z_i e (\Phi) / T_i}$ a pseudo-density and h_1 related to f_1 by

$$f_{i1} = h_1 - \frac{I v_{\parallel}}{\Omega_i} \frac{\partial f_{i0}}{\partial \psi} \Big|_E = h_1 - \frac{I v_{\parallel} f_{i0}}{\Omega_i} \left[\frac{1}{p_i} \frac{\partial p_i}{\partial \psi} + \frac{Z_i e}{T_i} \frac{\partial \Phi}{\partial \psi} + \left(\frac{M_i v^2}{2T_i} - \frac{5}{2} \right) \frac{1}{T_i} \frac{\partial T_i}{\partial \psi} \right]. \tag{4.3}$$

Evaluating the integrals for the explicit friction terms yields

$$\frac{3\sqrt{2\pi} T_i^{3/2} n_z}{2M_i^{3/2} n_i} \int d^3 v \frac{v_{\parallel} (f_{i1} - h_1)}{B v^3} = -\frac{c I n_z}{B^2} \frac{\partial \Phi}{\partial \psi} - \frac{c I n_z}{Z_i e n_i B^2} \left(\frac{\partial p_i}{\partial \psi} - \frac{3n_i}{2} \frac{\partial T_i}{\partial \psi} \right). \tag{4.4}$$

In the banana regime $v_{\parallel} \mathbf{b} \cdot \nabla h_1 = 0$ to lowest order making

$$u \equiv \frac{3\sqrt{2\pi} T_i^{3/2}}{2M_i^{3/2}} \int d^3 v \frac{v_{\parallel} h_1}{B v^3}, \tag{4.5}$$

a flux function. The trapped ion portion of h_1 vanishes as can be seen by transit averaging the next order kinetic equation and noting v_{\parallel} changes sign upon reflection. Then the terms (3.14) on the right side of the parallel momentum equation combine to give

$$\begin{aligned} \frac{n_z V_{\parallel z}}{B} - \frac{3\sqrt{2\pi} T_i^{3/2} n_z}{2M_i^{3/2} n_i} \int d^3 v \frac{v_{\parallel} f_{i1}}{B v^3} &= K_z - \frac{n_z u}{n_i} + \frac{cI}{Z_z e B^2} \frac{\partial}{\partial \psi} [\alpha \langle p_z \rangle (n - 1) - \langle p_z \rangle] \\ &+ \frac{cI n_z}{Z_i e n_i B^2} \left(\frac{\partial p_i}{\partial \psi} - \frac{3n_i}{2} \frac{\partial T_i}{\partial \psi} \right). \end{aligned} \tag{4.6}$$

In addition, the radial particle flux is

$$\begin{aligned} Z_i \langle n_i V_i \cdot \nabla \psi \rangle &= -\frac{cI}{e} \left\langle \frac{F_{iz}^{\parallel}}{B} \right\rangle \\ &= -\frac{cI M_i n_i \langle v_{iz} \rangle}{e \langle n_z \rangle} \left\{ K_z - \frac{\langle n_z \rangle u}{n_i} + \frac{cI}{Z_z e} \left\langle \frac{1}{B^2} \frac{\partial}{\partial \psi} [\alpha \langle p_z \rangle (n - 1) - \langle p_z \rangle] \right\rangle \right. \\ &\quad \left. + \frac{cI}{Z_i e n_i} \left\langle \frac{n_z}{B^2} \right\rangle \left(\frac{\partial p_i}{\partial \psi} - \frac{3n_i}{2} \frac{\partial T_i}{\partial \psi} \right) \right\}. \end{aligned} \tag{4.7}$$

Defining the gradient flux function G by

$$G = G(\psi) = -\frac{cIM_i\langle v_{iz} \rangle}{Z_i e \langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle} \left(\frac{\partial p_i}{\partial \psi} - \frac{3n_i}{2} \frac{\partial T_i}{\partial \psi} \right), \quad (4.8)$$

an impurity diamagnetic flux function $D \propto 1/Z_z$ by

$$D = D(\psi) = -\frac{cIM_i n_i \langle v_{iz} \rangle}{Z_z e \langle p_z \rangle \langle n_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle} \frac{\partial \langle p_z \rangle}{\partial \psi}, \quad (4.9)$$

a poloidal flow flux function

$$K = K(\psi) = \frac{M_i n_i \langle v_{iz} \rangle \langle B^2 \rangle}{\langle p_z \rangle \langle n_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle} K_z, \quad (4.10)$$

and a flow quantity U (that is only a flux function in the banana regime)

$$U = \frac{M_i \langle v_{iz} \rangle \langle B^2 \rangle u}{\langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle}, \quad (4.11)$$

then the parallel impurity momentum equation in the banana regime becomes

$$(1 + \alpha n) \frac{\partial n}{\partial \theta} = Gn - Kb^2 + Unb^2 - D \left\{ 1 - \frac{\partial [\alpha \langle p_z \rangle (n - 1)] / \partial \psi}{\partial \langle p_z \rangle / \partial \psi} \right\}. \quad (4.12)$$

To obtain the last term it is necessary to make an aspect ratio expansion, (3.22), but the other terms are valid for general B and n_z . Notice that the final term in the expression multiplying D vanishes to lowest order upon flux surface averaging. Except for the generalization to include poloidal variation due to impurity diamagnetic effects, the orderings used here are essentially the same as Helander (1998) and Landreman *et al.* (2011) who ignore the impurity diamagnetic term D by assuming very large Z_z/Z_i . The treatment here retains D to lowest order in the parallel impurity momentum equation. Consequently, moderate $Z_z/Z_i \gg 1$ such as carbon and boron are allowed, and very large Z_z/Z_i (e.g. tungsten) need not be assumed.

Helander (1998), Landreman *et al.* (2011) and the treatment herein allow

$$G \sim \frac{\rho_{ip}}{L_\perp} \frac{Z_z^2}{Z_i^2} \frac{qRv_{ii}}{v_i} \sim 1, \quad (4.13)$$

where the poloidal ion gyroradius, $\rho_{ip} = v_i B / \Omega_i B_p$, is assumed much smaller than the radial scale length L_\perp . At the banana–plateau transition $G \sim (\rho_{ip}/L_\perp) (Z_z/Z_i)^2 \varepsilon^{3/2}$, indicating that for $G \sim 1$, $(Z_z/Z_i)^2 \varepsilon^{3/2} \gg 1$ is required.

Recalling that in the banana regime the quantity U is a flux function, the solubility constraint

$$K = G + U \langle nb^2 \rangle - D, \quad (4.14)$$

can be employed to eliminate K to find

$$(1 + \alpha n) \frac{\partial n}{\partial \theta} = G(n - b^2) + Ub^2(n - \langle nb^2 \rangle) - D \left\{ 1 - b^2 - \frac{\partial [\alpha \langle p_z \rangle (n - 1)] / \partial \psi}{\partial \langle p_z \rangle / \partial \psi} \right\}, \quad (4.15)$$

(which agrees with Helander (1998) when $Z_z \rightarrow \infty$). The orderings assume $D/G \sim Z_i/Z_z \ll 1$. The D term assumes $\varepsilon \ll 1$ and enters because then $D(1 - b^2)/G(n - b^2) \sim$

$Z_i/\varepsilon Z_z \sim 1$ is allowed. Measurements on Alcator C-Mod (Theiler *et al.* 2014) for $B_i > 0$ indicate $K > 0$ and $D > 0$ over most of the pedestal in both H and I modes. In I mode $\eta_i \equiv d\ln T_i/d\ln n_i > 2$ is expected, giving $G < 0$ in C-Mod and the flow term $U > 0$ in the banana regime. In H mode $\eta_i < 2$ is anticipated giving $G > 0$ in C-Mod, so U can be of either sign.

CXRS can measure impurity flow as well as impurity density and temperature variations. Therefore, it is useful to use solubility to eliminate U instead of K to rewrite the parallel impurity momentum equation in the banana regime as

$$(1 + \alpha n) \frac{\partial n}{\partial \theta} = G \left(n - \frac{nb^2}{\langle nb^2 \rangle} \right) - K \left(b^2 - \frac{nb^2}{\langle nb^2 \rangle} \right) + D \left[(n - 1) + (b^2 - 1) + \frac{\partial[\alpha \langle p_z \rangle (n - 1)]/\partial \psi}{\partial \langle p_z \rangle / \partial \psi} \right], \quad (4.16)$$

which generalizes the $Z_z \rightarrow \infty$ form in Espinosa & Catto (2017b) to include poloidal variation driven by the impurity pressure terms. To obtain this form, $Z_i/Z_z \sim \varepsilon$ is assumed to simplify the D term by using $nb^2/\langle nb^2 \rangle - b^2 \approx n - 1$. The orderings allow $G \sim 1 \sim K \sim Z_z D/Z_i$. For this ordering impurity pressure effects are only allowed to alter the poloidal variation of the impurity density by terms of order ε . For a realistic, strongly varying magnetic field, this equation could be solved numerically to find strong poloidal variation in the impurity density. However, at present, it seems highly unlikely that the various coefficients can be determined with the requisite certainty. Only a simple limiting solution will be given once the corresponding plateau regime equation is derived in the next section. In the weak gradient and flow, low confinement limit (L mode), the small up-down asymmetry satisfies $(1 + \alpha)\partial n/\partial \theta \approx G(1 - b^2)$ as in Helander (1998).

In addition to the poloidal impurity density variation, the particle flux can be evaluated for banana regime background ions from the friction. Using the same orderings

$$\frac{F_{iz}^{\parallel}}{B} = -\frac{\langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle}{\langle B^2 \rangle} \left\{ G \left(\frac{n}{b^2} - \frac{n}{\langle nb^2 \rangle} \right) - K \left(1 - \frac{n}{\langle nb^2 \rangle} \right) + D \left[\frac{n}{b^2} + 1 - \frac{2}{b^2} + \frac{\partial[\alpha \langle p_z \rangle (n - 1)]/\partial \psi}{b^2 \partial \langle p_z \rangle / \partial \psi} \right] \right\}. \quad (4.17)$$

The D term is negligible once (4.17) is averaged (recall it is derived assuming $\varepsilon \ll 1$) leading to the particle flux of banana regime background ions being

$$\langle n_i V_i \cdot \nabla \psi \rangle = -\frac{cI}{Z_i e} \left\langle \frac{F_{iz}^{\parallel}}{B} \right\rangle = \frac{cI \langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle}{Z_i e \langle B^2 \rangle} \left[G \left(\left\langle \frac{n}{b^2} \right\rangle - \frac{1}{\langle nb^2 \rangle} \right) - K \left(1 - \frac{1}{\langle nb^2 \rangle} \right) \right], \quad (4.18)$$

as in Espinosa & Catto (2017a,b, 2018) who also assume $T_i = T_z = \langle T_z \rangle$. This flux vanishes as desired for $n_z \rightarrow 0$. Also, large gradient ($G \gg 1$ and $D \gg 1$) and flow ($K \gg 1$) drives make the right side of (4.16) vanish and thereby reduces the friction, (4.17), and radial transport, (4.18), as pointed out by Helander (1998). When K is retained instead of U with $G = K \gg 1 \sim D$, (4.16) reduces to

$$G \left(n - \frac{nb^2}{\langle nb^2 \rangle} \right) \approx K \left(b^2 - \frac{nb^2}{\langle nb^2 \rangle} \right), \quad (4.19)$$

indicating that for $G > 0$ and $K > 0$ ($G < 0$ and $K < 0$) impurity accumulation will be large on the high field side (HFS), while impurity accumulation will occur on the LFS when

G and K are of opposite sign. The general form (4.17) and the approximate form (4.19) allow strong poloidal variation in the magnetic field and impurity density. For example, (4.19) can be solved for a specified b^2 by defining $g \equiv G/K$ to obtain the lowest-order result

$$n = b^2/[g + (1 - g)b^2/\langle nb^2 \rangle], \tag{4.20}$$

for a fixed g . The constant $\langle nb^2 \rangle$ is determined implicitly from the constraint

$$\langle b^2/[g + (1 - g)b^2/\langle nb^2 \rangle] \rangle = 1. \tag{4.21}$$

The special case $g = 1$ gives $n = b^2$ to lowest order. It allows (4.16) to be solved to next order to find $n = b^2 + K^{-1}[(1 + \alpha b^2)\partial b^2/\partial\theta - D(b^2 - 1)(2 + \partial\langle p_z \rangle/\partial\psi)^{-1}\partial(\alpha\langle p_z \rangle)/\partial\psi]$, demonstrating impurity diamagnetic modifications occur for $G = K \gg D \sim 1$.

The plateau regime parallel momentum equation and particle flux for the impurities are derived next in order that approximate solutions can be presented in a more streamlined and coordinated fashion.

5. Plateau regime background ions

In the plateau regime ($1 > v_{ii}qR/v_i > \varepsilon^{3/2}$) the form of the unlike collision operator $C_{iz}\{f_{i1}\}$ makes it necessary to let

$$f_{i1} = H_1 + \frac{M_i}{T_i} V_{||z} v_{||} f_{i0}, \tag{5.1}$$

with H_1 and h_1 related by

$$h_1 - H_1 = \frac{I v_{||}}{\Omega_i} \frac{\partial f_{i0}}{\partial \psi} \Big|_E + \frac{M_i}{T_i} V_{||z} v_{||} f_{i0}, \tag{5.2}$$

and, unlike the banana regime, $v_{||} \mathbf{b} \cdot \nabla h_1 \neq 0$. Then the plateau regime background ion kinetic equation to be solved for $\varepsilon \ll 1$ is

$$v_{||} \mathbf{b} \cdot \nabla \vartheta \frac{\partial H_1}{\partial \vartheta} - C_1\{H_1\} = -v_{||} \mathbf{b} \cdot \nabla \vartheta \left(\frac{I v_{||}}{\Omega_i} \frac{\partial f_{i0}}{\partial \psi} \Big|_E + \frac{M_i}{T_i} V_{||z} v_{||} f_{i0} \right). \tag{5.3}$$

In addition, the parallel impurity momentum equation to be solved for $\varepsilon \ll 1$ is

$$(1 + \alpha n) \frac{\partial n}{\partial \theta} = - \frac{BF_{iz}^{||}}{\langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle} = \frac{3\sqrt{2\pi} T_i^{3/2} v_{iz} B}{2M_i^{1/2} \langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle} \int d^3 v \frac{v_{||} H_1}{v^3}. \tag{5.4}$$

Solving in the plateau regime involves subtleties that need to be explained in some detail as the procedure used here differs from that of Landreman *et al.* (2011) as they assume differences in poloidal variation are unimportant by making the replacement $V_{||z} \rightarrow -(cI/Z_i e B n_i)[\partial p_i/\partial\psi + Z_i e n_i \partial\Phi/\partial\psi + (y b^2 n_i/2)\partial T_i/\partial\psi] \equiv V_{||i}^{\text{plat}}$. They assume very large Z_z so no $\langle p_z \rangle$ terms enter, and determine y from ambipolarity to recover $V_{||i}^{\text{plat}}$, which is the usual plateau expression (Hinton & Hazeltine 1976) for the parallel ion flow when $y = 1$.

For a plateau regime to exist $\varepsilon \approx r/R_0 \ll 1$ is required, where R_0 is the major radius of the magnetic axis. In addition to $d\theta = \langle \mathbf{B} \cdot \nabla \vartheta \rangle d\vartheta / \mathbf{B} \cdot \nabla \vartheta$ and $\mathbf{B} = B_0(1 - \varepsilon \cos \theta + \dots)$, with $B_0^2 = \langle B^2 \rangle$ and $\langle \mathbf{B} \cdot \nabla \vartheta \rangle \approx B_0/qR_0$, a large aspect ratio form for n ,

$$n = 1 + \varepsilon(n_c \cos \theta + n_s \sin \theta), \tag{5.5}$$

must be employed in the drive terms $K_z \partial(Bn_z^{-1})/\partial\theta$, $(\partial \langle p_z \rangle / \partial \psi) \partial(Bn_z)^{-1} / \partial\theta$ and $[(\partial/\partial\psi)\alpha \langle p_z \rangle \partial(n-1)/\partial\theta]$ of $V_{||z}$. Here, n_c and n_s are coefficients that will be determined by solving (5.4). Then the plateau regime kinetic equation is written as

$$v_{||} \frac{\partial H_1}{\partial \vartheta} - qR_0 C_1 \{H_1\} = Q_s \sin \theta + Q_c \cos \theta, \tag{5.6}$$

where θ dependence enters only via $\sin \theta$ and $\cos \theta$. In the preceding

$$Q_s = \frac{\varepsilon M_i}{2T_i} \left\{ \frac{cI(v_{\perp}^2 + 2v_{||}^2)}{Z_i e B_0 n_i} \left[\frac{\partial p_i}{\partial \psi} - \frac{Z_i n_i}{Z_z \langle n_z \rangle} \frac{\partial \langle p_z \rangle}{\partial \psi} + \left(\frac{M_i v^2}{2T_i} - \frac{5}{2} \right) n_i \frac{\partial T_i}{\partial \psi} \right] \right. \\ \left. + \frac{K_z B_0}{\langle n_z \rangle} [v_{\perp}^2 - 2(1 + n_c)v_{||}^2] + \frac{2cIv_{||}^2}{Z_z e B_0 \langle n_z \rangle} \left[n_c \frac{\partial \langle p_z \rangle}{\partial \psi} + \frac{\partial}{\partial \psi} (\alpha \langle p_z \rangle n_c) \right] \right\} f_{i0}, \tag{5.7}$$

and

$$Q_c = -\frac{\varepsilon M_i}{T_i} \left\{ \frac{cI}{Z_z e B_0 \langle n_z \rangle} \left[n_s \frac{\partial \langle p_z \rangle}{\partial \psi} + \frac{\partial}{\partial \psi} (\alpha \langle p_z \rangle n_s) \right] - \frac{K_z B_0}{\langle n_z \rangle} n_s \right\} v_{||}^2 f_{i0}. \tag{5.8}$$

Even in the $Z_z \rightarrow \infty$ limit, the poloidal variation of the impurity density matters and enters through the $K_z n_c$ and $K_z n_s$ terms. In the plateau regime, most ions are collisionless requiring $qRv_{ii}/v_i \ll 1$. Nevertheless, collisions must be strong enough that no ions are trapped. The ξ boundary layer width ξ_w is found by balancing streaming with collisions, $\xi_w v_i \sim v_{ii} qR / \xi_w^2$, to find the plateau ordering $1 \gg \xi_w \sim (v_{ii} qR / v_i)^{1/3} \gg \varepsilon^{1/2}$, with $\varepsilon^{1/2}$ the trapped fraction.

Once the kinetic equation is in the proper form for the plateau regime the details of the collision operator do not matter in most situations. However, to check, the unlike collision operator (3.11) is used for ion–impurity collisions and the following momentum conserving, model ion–ion collisions operator is employed

$$C_{ii}\{f_{i1}\} = \frac{3\sqrt{\pi}T_i^{3/2}v_{ii}}{2M_i^{3/2}} \nabla_v \cdot \left[\nabla_v \nabla_v v \cdot \nabla_v \left(f_{i1} - \frac{M_i}{T_i} W_{||i} v_{||} f_{i0} \right) \right], \tag{5.9}$$

with $W_{||i} = 3T_i \int d^3 v v_{||} v^{-3} f_{i1} / M_i \int d^3 v v^{-1} f_{i0}$, and, for $v_{||} = \xi v$,

$$\nabla_v \cdot (\nabla_v \nabla_v v \cdot \nabla_v f) = v^{-3} \frac{\partial}{\partial \xi} \left[(1 - \xi^2) \frac{\partial f}{\partial \xi} \right]. \tag{5.10}$$

Only the diffusive terms matter in the plateau regime, giving

$$C_1\{H_1\} = v \frac{\partial}{\partial \xi} \left[(1 - \xi^2) \frac{\partial H_1}{\partial \xi} \right] \approx v \frac{\partial^2 H_1}{\partial \xi^2}, \tag{5.11}$$

with

$$v = \frac{3\sqrt{2\pi}T_i^{3/2}}{4M_i^{3/2}v^3} (\sqrt{2}v_{ii} + v_{iz}). \tag{5.12}$$

Then the plateau kinetic equation in v, ξ variables becomes

$$\xi v \frac{\partial H_1}{\partial \vartheta} - \nu q R_0 \frac{\partial^2 H_1}{\partial \xi^2} = \text{Im}\{(Q_s + iQ_c) e^{i\theta}\}, \tag{5.13}$$

where the mirror force term, $\varepsilon \mu B_0 v^{-1} \sin \theta \partial H_1 / \partial \xi \sim \varepsilon v H_1 / \xi_w$, is negligible compared with $\xi v \partial H_1 / \partial \vartheta \sim \xi_w v H_1$ in the ξ boundary layer of width ξ_w since $\varepsilon (v_i / v_{ii} q R)^{2/3} \ll 1$.

The flux function K_z must be chosen in a manner ensuring ion transport vanishes in the absence of impurities. It is tempting to think of the ion-impurity transport problem as being very much the same as the electron-ion transport problem. Nonetheless, there are important and subtle differences. In particular, impurity collisions cannot modify the ion distribution function when $n_z \rightarrow 0$, while the electron distribution is always modified by the ion collisions (see the Appendix of Pusztai & Catto (2010) for a summary of the electron-ion treatment).

Letting $u = \gamma \xi$, defining

$$\gamma = (\nu / \nu q R_0)^{1/3} \gg 1, \tag{5.14}$$

and noting that the localized solution to $\partial^2 h / \partial u^2 - i u h = -1$ is $h = \int_0^\infty dx e^{-x^3/3 - i u x}$, the plateau kinetic equation solution is found to be

$$\begin{aligned} H_1 &= \frac{\gamma}{v} \text{Im} \left\{ (Q_s + iQ_c) e^{i\theta} \int_0^\infty dx e^{-x^3/3 - i \gamma \xi x} \right\} \\ &= \frac{\gamma Q_s}{v} \left[\sin \theta \int_0^\infty dx e^{-x^3/3} \cos(\gamma \xi x) - \cos \theta \int_0^\infty dx e^{-x^3/3} \sin(\gamma \xi x) \right] \\ &\quad + \frac{\gamma Q_c}{v} \left[\cos \theta \int_0^\infty dx e^{-x^3/3} \cos(\gamma \xi x) + \sin \theta \int_0^\infty dx e^{-x^3/3} \sin(\gamma \xi x) \right], \end{aligned} \tag{5.15}$$

where all $\xi \lesssim \sqrt{\varepsilon}$ ions are collisional and $\xi \sim 1$ ions are collisionless. For this solution

$$\gamma \int_{-1}^1 d\xi \int_0^\infty dx e^{-x^3/3} \cos(\gamma \xi x) = 2 \int_0^\infty \frac{dx}{x} e^{-x^3/3} \sin(\gamma x) \xrightarrow{\gamma \gg 1} \pi, \tag{5.16}$$

implying

$$\gamma \int_0^\infty dx e^{-x^3/3} \cos(\gamma \xi x) \xrightarrow{\gamma \gg 1} \pi \delta(\xi), \tag{5.17}$$

while

$$\gamma \int_{-1}^1 d\xi \int_0^\infty dx e^{-x^3/3} \sin(\gamma \xi x) = - \int_0^\infty \frac{dx}{x} e^{-x^3/3} \int_{-1}^1 d\xi \frac{d}{d\xi} \cos(\gamma \xi x) = 0, \tag{5.18}$$

and

$$\gamma \int_0^\infty dx e^{-x^3/3} \sin(\gamma \xi x) = - \frac{1}{\xi} \int_0^\infty dx e^{-x^3/3} \frac{d}{dx} \cos(\gamma \xi x) \xrightarrow{\gamma \gg 1} \frac{1}{\xi}. \tag{5.19}$$

To evaluate the integrals needed here all that is required is

$$H_1 = Q_s \left[\frac{\pi}{v} \delta(\xi) \sin \theta - \frac{\cos \theta}{v_{||}} \right] + Q_c \left[\frac{\pi}{v} \delta(\xi) \cos \theta + \frac{\sin \theta}{v_{||}} \right], \tag{5.20}$$

implying the replacement $C_1\{H_1\} \rightarrow -\nu_{\text{eff}} H_1$ with $\nu_{\text{eff}} \sim \nu / \xi_w^2$ can be employed in (5.6).

Only H_1 terms odd in $v_{||}$ contribute to the friction giving

$$\int d^3v \frac{v_{||} H_1}{v^3} = \sin \theta \int d^3v \frac{Q_c}{v^3} - \cos \theta \int d^3v \frac{Q_s}{v^3}, \quad (5.21)$$

where

$$\int d^3v \frac{Q_c}{v^3} = \varepsilon \frac{2M_i^{3/2} n_i B_0}{3\sqrt{2\pi} T_i^{3/2} \langle n_z \rangle} \left\{ n_s K_z - \frac{cI}{Z_c e B_0^2} \left[n_s \frac{\partial \langle p_z \rangle}{\partial \psi} + \frac{\partial}{\partial \psi} (\alpha \langle p_z \rangle n_s) \right] \right\}, \quad (5.22)$$

and

$$\begin{aligned} \int d^3v \frac{Q_s}{v^3} = & \varepsilon \frac{4cIM_i^{3/2}}{3\sqrt{2\pi} Z_i e T_i^{3/2} B_0} \left(\frac{\partial p_i}{\partial \psi} - \frac{Z_i n_i}{Z_c \langle n_z \rangle} \frac{\partial \langle p_z \rangle}{\partial \psi} - \frac{3}{2} n_i \frac{\partial T_i}{\partial \psi} \right) \\ & - \varepsilon \frac{2M_i^{3/2} n_i B_0}{3\sqrt{2\pi} T_i^{3/2} \langle n_z \rangle} \left\{ n_c K_z - \frac{cI}{Z_c e B_0^2} \left[n_c \frac{\partial \langle p_z \rangle}{\partial \psi} + \frac{\partial}{\partial \psi} (\alpha \langle p_z \rangle n_c) \right] \right\}, \end{aligned} \quad (5.23)$$

where $\partial \varepsilon / \partial \psi \approx 1/R_0^2 B_p = q/rR_0 B_0$ terms are ignored as unimportant compared with those varying on the radial scale of the pedestal and $\langle B^{-1} \int d^3v v^{-3} v_{||} H_1 \rangle = 0$ for any plateau regime solution. As a result, the parallel impurity momentum equation to order ε for plateau regime background ions is

$$(1 + \alpha n) \frac{\partial n}{\partial \theta} = 2\varepsilon(G - D) \cos \theta + (K + D)(n - 1) + D \frac{\partial[\alpha \langle p_z \rangle (n - 1)] / \partial \psi}{\partial \langle p_z \rangle / \partial \psi}; \quad (5.24)$$

exactly the same as for banana regime background ions when $\varepsilon \ll 1$ and (5.5) is inserted, implying that (4.16) can be used for both regimes! All D terms are local, except $\partial(n - 1)/\partial \psi$. The solution n is also local since it depends on radial first derivatives. However, $\partial(n - 1)/\partial \psi$ is non-local as it implicitly leads to second derivatives in radius. The full expression for the D terms was not recovered in the Espinosa & Catto (2019) due to a less accurate treatment of the parallel friction; and because their (8) ignores radial derivatives and it is used in their (46) and (50) to obtain (51) (they also order the poloidal variation of the impurity density as stronger than the poloidal variation of B).

6. Approximate solutions for impurity density variation and radial particle transport

The parallel impurity momentum equation can be solved in detail if all radial profiles are accurately known, but as they are often not, it seems wisest to give a useful approximate solution for $Z_i/Z_c \lesssim \varepsilon \ll 1$. As $G \sim 1 \sim K \sim Z_c D/Z_i$, in this limit the lowest order parallel impurity momentum equation is simply

$$(1 + \alpha n) \frac{\partial n}{\partial \theta} = 2\varepsilon G \cos \theta + K(n - 1), \quad (6.1)$$

and the solution for both banana and plateau regime background ions is

$$n = 1 + 2\varepsilon G \frac{(1 + \alpha) \sin \theta - K \cos \theta}{(1 + \alpha)^2 + K^2}. \quad (6.2)$$

The clear features of the solution are that the sign of G determines the up–down asymmetry. The in–out asymmetry depends on the sign and size of both K and G , where

the sign of the flux surface averaged poloidal flow gives the sign of K ,

$$\frac{\langle n_z \mathbf{V}_z \cdot \nabla \vartheta \rangle}{\langle \mathbf{B} \cdot \nabla \vartheta \rangle} \approx K_z(\psi) = \frac{\langle p_z \rangle \langle n_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle}{M_i n_i \langle v_{iz} \rangle \langle B^2 \rangle} K, \quad (6.3)$$

as $\nabla \vartheta$ and $\nabla \zeta \times \nabla \psi$ are roughly in the same direction and $\mathbf{B} \cdot \nabla \vartheta \approx \langle \mathbf{B} \cdot \nabla \vartheta \rangle$ to lowest order. A solution for n retaining impurity diamagnetic effects when $1 \gg Z_i/Z_e \gg \varepsilon$ is given in [Appendix A](#) and further illustrates the need for radial profile information.

6.1. Banana regime transport

The large aspect ratio background ion particle flux for banana regime ions colliding with impurities is

$$\langle n_i \mathbf{V}_i \cdot \nabla \psi \rangle = \varepsilon^2 \frac{cI \langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle}{Z_i e \langle B^2 \rangle} (2G + n_c K) = \frac{2\varepsilon^2 cI (1 + \alpha)^2 \langle p_z \rangle \langle \mathbf{B} \cdot \nabla \vartheta \rangle G}{Z_i e \langle B^2 \rangle [(1 + \alpha)^2 + K^2]}, \quad (6.4)$$

as $\langle nb^{-2} \rangle - 1 = \langle (b^2 - 1)^2 b^{-2} \rangle - \langle (n - 1)(b^2 - 1)b^{-2} \rangle \approx (2 + n_c)\varepsilon^2$, $\langle nb^2 \rangle - 1 = \langle (n - 1)(b^2 - 1) \rangle \approx -n_c \varepsilon^2$, $\langle nb^{-2} \rangle - \langle nb^2 \rangle^{-1} \approx 2\varepsilon^2$ and $K = G + \langle nb^2 \rangle U + D \approx G + U$. Consequently, the direction of the radial ion particle flux for banana regime background ions depends on the sign of $IG \propto -I^2(2T_i \partial n_i / \partial \psi - n_i \partial T_i / \partial \psi)$, while the direction of the poloidal flow is unimportant as only K^2 enters to reduce the transport. When $IG > 0$ or $\eta_i = d\ell n T_i / d\ell n n_i < 2$ (as in H mode) the background ion particle flux is outward, while for $IG < 0$ or $\eta_i = d\ell n T_i / d\ell n n_i > 2$ (as in I mode) the background ions are transported inward ([Churchill et al. 2015](#)) and provide natural fuelling. This desirable $\eta_i > 2$ case is sometimes referred to as temperature screening because the radial flux of impurities is outward ([Wade, Houlberg & Baylor 2000](#)).

6.2. Plateau regime transport

The lowest order expression for the friction used to obtain the parallel impurity momentum equation for plateau regime background ions is not good enough to evaluate the particle flux since $\langle n_z \mathbf{V}_z \cdot \nabla \psi \rangle = (cI/Z_e) \langle F_{iz}^{\parallel} / B \rangle = 0$. As a result, the particle flux for plateau regime ions is negligibly small and K_z must be found from

$$\langle n_i \mathbf{V}_i \cdot \nabla \psi \rangle = \left\langle \int d^3 v f_{i1} \mathbf{v}_d \cdot \nabla \psi \right\rangle = \left\langle \int d^3 v H_1 \mathbf{v}_d \cdot \nabla \psi \right\rangle, \quad (6.5)$$

where

$$\mathbf{v}_d \cdot \nabla \psi = I v_{\parallel} \mathbf{b} \cdot \nabla \left(\frac{v_{\parallel}}{\Omega_i} \right) \Big|_{E,\mu} \approx -\frac{\varepsilon M_i c}{2Z_i e q} (v_{\perp}^2 + 2v_{\parallel}^2) \sin \theta, \quad (6.6)$$

as the poloidal variation of the potential is very weak. Evaluating the integrals by noting only the sin terms even in v_{\parallel} contribute, with $\langle \sin^2 \theta \rangle = 1/2$ and $d^3 v = 2\pi v^2 dv d\xi$, yields

$$\begin{aligned} \langle n_i \mathbf{V}_i \cdot \nabla \psi \rangle &= -\frac{\pi \varepsilon M_i c}{4Z_i e q} \int d^3 v v \delta(\xi) Q_s \\ &= -\frac{\sqrt{2\pi} \varepsilon^2 I B_0 T_i^{3/2} n_i}{2q \Omega_0^2 M_i^{3/2}} \left(\frac{1}{p_i} \frac{\partial p_i}{\partial \psi} - \frac{Z_i}{Z_e \langle p_z \rangle} \frac{\partial \langle p_z \rangle}{\partial \psi} + \frac{1}{2T_i} \frac{\partial T_i}{\partial \psi} + \frac{Z_i e B_0^2}{cI \langle p_z \rangle} K_z \right), \end{aligned} \quad (6.7)$$

where $\Omega_0 = Z_i e B_0 / M_i c$. The main ion density and temperature gradient terms give a plateau diffusivity of $q v_i^3 / \Omega_0^2 R$ (which is $M_i^{1/2} / M_e^{1/2} \gg 1$ larger than the electron particle diffusivity).

Comparing the size of the $\partial p_i / \partial \psi$ terms from both ways of evaluating the particle flux and accounting for $\langle F_{iz}^{\parallel} / B \rangle = 0$ leads to

$$[(cI/Z_i e) \langle F_{iz}^{\parallel} / B \rangle] / \left\langle \int d^3 v H_1 \mathbf{v}_d \cdot \nabla \psi \right\rangle \ll v_{iz} q R_0 / \varepsilon v_i \sim \alpha v_{iz} q R_0 / \varepsilon v_i, \quad (6.8)$$

where electron transport is assumed negligible, $\alpha \lesssim 1$ and $\sqrt{\varepsilon} < v_{iz} q R_0 / \varepsilon v_i < 1/\varepsilon$ in the plateau regime. The preceding estimate indicates the need to use $\langle \int d^3 v H_1 \mathbf{v}_d \cdot \nabla \psi \rangle$ to evaluate K_z .

Based on the preceding estimates and the need to maintain ambipolarity between the ions and the impurities, the radial ion particle transport must vanish to lowest order

$$\langle n_i \mathbf{V}_i \cdot \nabla \psi \rangle \approx 0, \quad (6.9)$$

thereby determining K_z to be given by

$$\frac{1}{p_i} \frac{\partial p_i}{\partial \psi} - \frac{Z_i}{Z_e \langle p_z \rangle} \frac{\partial \langle p_z \rangle}{\partial \psi} + \frac{1}{2T_i} \frac{\partial T_i}{\partial \psi} + \frac{Z_i e \langle B^2 \rangle}{cI \langle p_z \rangle} K_z = 0. \quad (6.10)$$

Again, friction seems to be acting reduce the neoclassical particle flux.

Ignoring poloidally varying terms, the preceding inserted in (3.28) leads to the lowest order relation between the parallel impurity and background ion flows

$$V_{\parallel z} \approx -\frac{cI}{B} \frac{\partial \Phi}{\partial \psi} - \frac{cIB}{Z_i e \langle B^2 \rangle n_i} \left(\frac{\partial p_i}{\partial \psi} + \frac{n_i}{2} \frac{\partial T_i}{\partial \psi} \right) \approx V_{\parallel i}^{\text{plat}}, \quad (6.11)$$

where $V_{\parallel i}^{\text{plat}}$ is the usual plateau expression for the parallel ion flow (Hinton & Hazeltine 1976). All the poloidally varying terms can be evaluated by using $n_i V_{\parallel i} = \int d^3 v v_{\parallel} f_{i1}$ to obtain the full relation between the parallel ion and impurity flows in the plateau regime

$$V_{\parallel i} - V_{\parallel z} = n_i^{-1} \int d^3 v v_{\parallel} H_1 = n_i^{-1} \left(\sin \theta \int d^3 v Q_c - \cos \theta \int d^3 v Q_s \right) \sim \varepsilon v_i \rho_{ip} / L_{\perp}, \quad (6.12)$$

but as there are many terms and they are small in ε they are not given here. These terms account for the difference between the results here and Landreman *et al.* (2011) for $Z_z \rightarrow \infty$.

Using the preceding expression for $V_{\parallel z}$ gives a consistency check on the lowest order plateau regime poloidal impurity flow to be

$$\begin{aligned} \frac{\langle n_z \mathbf{V}_z \cdot \nabla \vartheta \rangle}{\langle \mathbf{B} \cdot \nabla \vartheta \rangle} &\approx K_z(\psi) = -\frac{cI \langle p_z \rangle}{Z_i e \langle B^2 \rangle} \left(\frac{1}{p_i} \frac{\partial p_i}{\partial \psi} - \frac{Z_i}{Z_e \langle p_z \rangle} \frac{\partial \langle p_z \rangle}{\partial \psi} + \frac{1}{2T_i} \frac{\partial T_i}{\partial \psi} \right) \\ &\approx -\frac{cI \langle p_z \rangle}{Z_i e \langle B^2 \rangle} \left(\frac{1}{p_i} \frac{\partial p_i}{\partial \psi} + \frac{1}{2T_i} \frac{\partial T_i}{\partial \psi} \right). \end{aligned} \quad (6.13)$$

On Alcator C-Mod a positive poloidal flow, $K > 0$, is typically observed when $I > 0$ (Theiler *et al.* 2014). In AUG when $I < 0$, a negative poloidal flow, $K < 0$, occurs (Viezzler *et al.* 2013a; Cruz-Zabala *et al.* 2022).

The plateau solution in Landreman *et al.* (2011) is sensibly formulated to recover the standard result without impurities, but to do so it assumes $K_z/n_z = -y(cI/2Z_i e \langle B^2 \rangle) \partial T_i / \partial \psi$ in $V_{||z}$ with the parameter y determined by ambipolarity. Their procedure replaces $V_{||z}$ by $V_{||i}$ in f_{i1} so does not properly account for various poloidally varying drive terms in $C_{iz} \{ (V_{||z} - V_{||i}) v_{||i} f_{i0} \} \neq 0$, and thereby misses impurity density drive terms such as $K_z \partial (B n_z^{-1}) / \partial \theta$ which require writing $n = 1 + \varepsilon (n_c \cos \theta + n_s \sin \theta)$. Moreover, like all plateau regime treatments, Landreman *et al.* (2011) should only find H_1 to lowest order in ε and be unable to evaluate the radial flux from the friction as $\langle F_{iz}^{||} / B \rangle = 0$.

7. Diffusion and convection form of impurity continuity

To cast the impurity continuity equation into the popular diffusion and convection form

$$\frac{\partial \langle n_z \rangle}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(D_z \frac{\partial \langle n_z \rangle}{\partial r} - V_z \langle n_z \rangle \right) \right], \tag{7.1}$$

for banana regime background ions and trace impurities, the small term D must be retained in (4.18) by making the replacement $G \rightarrow G - D$, as suggested by (4.12) and (6.7). Of course, the orderings used here imply the particle diffusivity term D_z is less important than the radial convection velocity V_z . Using ambipolarity gives the impurity flux as $\langle n_z V_z \cdot \nabla \psi \rangle = -Z_i \langle n_i V_i \cdot \nabla \psi \rangle / Z_z \approx -RB_p (D_z \partial \langle n_z \rangle / \partial r - V_z \langle n_z \rangle)$, upon using the large aspect ratio approximation $RB_p \partial / \partial \psi \approx \partial / \partial r$ for $|\nabla \psi| = RB_p$. Then (6.4) leads to

$$D_z = \frac{2\varepsilon^2 c^2 M_i p_i \langle v_{iz} \rangle}{Z_z^2 e^2 B_p^2 \langle n_z \rangle (1 + K^2)}, \tag{7.2}$$

and

$$\frac{RV_z}{D_z} = -\frac{R}{T_i} \frac{\partial T_i}{\partial r} + \frac{Z_z}{Z_i} \left(\frac{R}{n_i} \frac{\partial n_i}{\partial r} - \frac{R}{2T_i} \frac{\partial T_i}{\partial r} \right) \approx \frac{Z_z}{Z_i} \left(\frac{R}{n_i} \frac{\partial n_i}{\partial r} - \frac{R}{2T_i} \frac{\partial T_i}{\partial r} \right), \tag{7.3}$$

where the diffusivity and the first term in RV_z/D_z are small by Z_i/Z_z . In the diffusion and convection form the outward diffusion ($\partial \langle n_z \rangle / \partial r < 0$) can be counteracted by a pinch ($V_z < 0$). Notice that the convection velocity changes sign at $\eta_i = 2$, with a pinch ($V_z < 0$) for $\eta_i < 2$, and $V_z > 0$ (outward) if $\eta_i > 2$. The direction of the poloidal flow is unimportant as only K^2 enters.

In the plateau regime the vanishing of the radial impurity diffusion determines the unknown flux function K_z , making the poloidal flow positive ($K > 0$). In this case it is not possible to write a diffusion–convection form of impurity continuity.

The treatment here and in Helander (1998) assumes that in the banana regime the time for the impurities to diffuse across the magnetic field, L_\perp^2/D_z , is large compared with the time for the impurities to equilibrate along the magnetic field, $q^2 R^2 v_{zz} / v_z^2$. The ratio yields a restriction

$$1 \gg \frac{q^2 R^2 v_{zz} / v_z^2}{L_\perp^2 / D_z} \sim \left(\frac{\rho_{ip} Z_z^2 q R v_{ii}}{L_\perp Z_i v_i} \right)^2 \frac{\varepsilon^2 \alpha}{(Z_z / Z_i)^{3/2}} \sim G^2 \frac{\varepsilon^2 \alpha}{(Z_z / Z_i)^{3/2}}, \tag{7.4}$$

consistent with allowing $G \sim 1$ as assumed, and slightly more forgiving than the inequality of Helander (1998) who uses $\varepsilon^2 \sim 1$. However, radial impurity convection is Z_z/Z_i faster than diffusion, making the restriction more severe by requiring $G^2 \varepsilon^2 \alpha \ll (Z_z/Z_i)^{1/2}$. In the plateau regime the time for the impurities to diffuse across the field is very long as the radial transport is negligible, so the impurities are more easily able to equilibrate along the magnetic field.

8. Summary of results

The pedestal model considered herein assumes the poloidal ion gyroradius is small compared with the radial pedestal scale lengths. Within this important limitation (Trinczek *et al.* 2023), a pedestal treatment is formulated and solved that evaluates the poloidal variation of the impurity density and electrostatic potential as related by (3.17). In addition, the radial transport of the background ions and impurities in both the banana and plateau regimes is evaluated with the impurity diamagnetic pressure term retained. Weak poloidal variation in the plasma density, (3.12) and (3.16), is also retained, but any poloidal variation of the equal ion and impurity temperatures is neglected. At large aspect ratio, when the subtleties of the plateau treatment are taken into account, the parallel impurity momentum equation, (5.24), is shown to be the same as in the banana regime. When the impurity diamagnetic terms are negligible, the banana regime treatment reduces to the original treatment of Helander (1998), with a gradient drive term and a second drive term that requires solving the perturbed ion kinetic equation, (4.1), and it also recovers the formulation of Espinosa & Catto (2017*a,b*, 2018), for which the drives are the gradient term (4.8) and a poloidal flow term, (4.10), a term that can be measured by CXRS (McDermott *et al.* 2009; Viezzer *et al.* 2013*a,b*; Theiler *et al.* 2014; Cruz-Zabala *et al.* 2022).

The new impurity pressure gradient drive terms have the coefficient defined by (4.9) and also account for the non-local behaviour due to drift departures from flux surfaces due to the poloidal variation of the impurity density. All the impurity pressure gradient effects are obtained by assuming the aspect ratio is large – an assumption that need not be made for the other terms in the banana regime, but of course, must always be made in the plateau regime. The impurity pressure gradient terms provide an additional source of poloidal impurity density variation as can be seen by examining (4.16) and (5.24). However, because $Z_i/Z_e \ll 1$ they do not significantly alter the radial transport and poloidal flow in the plateau regime or the large aspect ratio limit of the banana regime. The plateau regime results found here remove limitations of an earlier treatment (Landreman *et al.* 2011). Even with the inadequacies of the derivations herein, the neoclassical results derived for the particle transport and flows suggest useful means of checking them against experimental measurements even when the poloidal variation of the impurity density is not allowed to be strong. In the banana regime, when the gradient coefficient G and the poloidal flow coefficient K are order unity or larger, large poloidal impurity variation occurs for realistic magnetic fields, but only a large G and K solution is presented here. No attempt is made here to explain heat fluxes as they are expected to be a combination of neoclassical and $\mathbf{E} \times \mathbf{B}$ shear regulated turbulent processes (Viezzer *et al.* 2017, 2018). In addition, the collisional Pfirsch–Schlüter regime for the main ions is not considered as it requires $\rho_{ip}/L_\perp \ll v_i/qRv_{ii} \ll 1$, leading to different results (Fülöp & Helander 2001; Maget *et al.* 2020*a,b*). Some C -Mod H mode plasmas may be collisional enough to enter the Pfirsch–Schlüter regime (Theiler *et al.* 2014).

The signs of $I = RB_t$, G (the gradient drive term) and K (the poloidal flow drive term) vary depending on geometry and operation mode. Consequently, some notable results are summarized in Table 1 for the two directions of the toroidal magnetic field relative to the Ohmic current: aligned (co) and opposed (counter). The entries are largely based on (6.2), (6.3), (6.4), (6.9) and (6.13). Additional information follows from the general banana regime solution of Fülöp & Helander (1999) in the trace limit, for which

$$u \approx -\frac{0.33JIn_i}{M_i\Omega_0B_0} \frac{\partial T_i}{\partial \psi}, \quad (8.1)$$

$\eta_i < 2$ (H mode: deep potential well)		Model Predictions	$\eta_i > 2$ (I mode: modest potential well)	
co B_t ($I > 0, G > 0$)	counter B_t ($I < 0, G < 0$)		co B_t ($I > 0, G < 0$)	counter B_t ($I < 0, G > 0$)
Impurities inward Ions outward	Impurities inward Ions outward	Banana regime radial transport: Recall (6.4)	Impurities outward Ions inward	Impurities outward Ions inward
negligible	negligible	Plateau regime radial transport	negligible	negligible
co B_p since $K > 0$ (B14) implies $U > 0$ in $K = G + U$	counter B_p since $K < 0$ (B14) implies $U < 0$ in $K = G + U$	Poloidal impurity flow in banana regime	$V_p B_t > 0$ in (3.4) for $E_r < 0$ co B_p	$V_p B_t > 0$ in (3.4) for $E_r < 0$ counter B_p
co B_p since $K > 0$	counter B_p since $K < 0$	Poloidal impurity flow in plateau regime: recall (6.13)	co B_p since $K > 0$	counter B_p since $K < 0$
HFS since $K > 0$	HFS since $K < 0$	In-out impurity accumulation: banana and plateau	LFS since $K > 0$	LFS since $K < 0$
accumulation opposite $B \times \nabla B$ direction	accumulation opposite $B \times \nabla B$ direction	Up-down impurity accumulation: banana and plateau	accumulation in $B \times \nabla B$ direction	accumulation in $B \times \nabla B$ direction

TABLE 1. Co B_t denotes $B_t = I \nabla \zeta$ is in the direction of the Ohmic current, while counter B_t is in the opposite direction. H mode plasmas are assumed to have $\eta_i \equiv d \ln T_i / d \ln n_i < 2$, while I mode plasmas are assumed to satisfy $\eta_i \equiv d \ln T_i / d \ln n_i > 2$. High and low field sides are denoted by HFS and LFS, respectively. Equation (6.2) is used to determine in-out and up-down asymmetries. L mode plasmas do not have significant poloidal variation or flow so do not have an appreciable radial electric field in the pedestal. Notice the signs of the toroidal magnetic field direction I and the poloidal impurity flow K are expected to be the same based on the theory presented here and the I mode experimental observation that $V_p B_t > 0$ in (3.4) to make $E_r < 0$.

with $J \approx 1 - 1.46\sqrt{\varepsilon}$. A brief derivation of the trace limit is presented in [Appendix B](#). Based on this $\alpha \ll 1$ limit, $U/I > 0$ for a normal negative temperature gradient. Consequently, using the lowest order solubility constraint $K = G + U$, in the H mode limit the poloidal flow is expected to be in the direction of the poloidal magnetic field for $I = RB_t > 0$, and opposite to the poloidal magnetic field for $I = RB_t < 0$. In the I mode limit measurements in C -Mod (Theiler *et al.* 2014) and AUG (Viezza *et al.* 2013a) normally find $V_p B_t > 0$ (that is, $KI > 0$), except perhaps near the last closed flux surface, leading to co \mathbf{B}_p flow for $B_t > 0$ and counter \mathbf{B}_p for $B_t < 0$. In making [Table 1](#), the stronger density gradient limit ($\eta_i < 2$) is presumed to be H mode, while the weaker density gradient or temperature screening limit ($\eta_i > 2$) is assumed to be I mode (the weakest gradient limit is expected to be L mode and is not listed as the poloidal variation is very weak as G and K are thought to be very small). The table is based on the results presented here except for the experimental observation that the poloidal flow term in I mode makes a negative radial electric field contribution. It indicates in-out impurity accumulation is a key difference between H and I mode pedestals, while the sign of the toroidal magnetic field and the poloidal impurity flow are the same ($KI > 0$).

The simplest, large aspect ratio results obtained here can be qualitatively compared with experimental results. General aspect ratio results can be obtained from (4.20) and (4.21) for $|G| \gg 1$, where normally $g = G/K > 0$ in H mode and $G/K < 0$ is expected in I mode. In particular, Alcator C -Mod with $I = RB_t > 0$ measures a positive poloidal flow ($K > 0$) as well as a negative radial impurity pressure gradient ($D > 0$) in H and I mode (Theiler *et al.* 2014).

In H mode at Alcator C -Mod, the HFS impurity density is found to be larger than the LFS impurity density (Churchill *et al.* 2013, 2015) as expected. And from (3.17), the poloidal electric field becomes more negative on the LFS as the impurity density increases on the HFS. The model considered here is consistent with impurity temperature alignment since $T_i = T_z = \langle T_z \rangle$. And it is also consistent with total pressure, $p_e + p_i$, alignment. To see this, flux surface averaged quasineutrality, $\langle n_e \rangle = Z_i \langle n_i \rangle$, is used to find $p_e + p_i = n_e T_e + n_i T_i = \langle n_e \rangle [T_e + e(\Phi - \langle \Phi \rangle)] + n_i [T_i - Z_i e(\Phi - \langle \Phi \rangle)] = \langle n_i \rangle (Z_i T_e + T_i)$, where T_e and T_i are flux functions. Interestingly, the impurity temperature alignment gives a nice match of profiles, possibly indicating that ion pressure anisotropy is spoiling total pressure alignment. However, the radial relation between $\Phi - \langle \Phi \rangle$ and $n_z - \langle n_z \rangle$ must also satisfy (3.17), and it is not apparent which alignment is better. Also, the poloidal variations are stronger than the large aspect ratio expansions often used here allow, and there may be some poloidal variation in the impurity temperature.

The poloidal variations in AUG are weaker than in C -Mod. Also, in AUG when $I = RB_t < 0$ and the poloidal flow is negative in H (as expected) and I modes (Viezza *et al.* 2013a). In H mode at AUG, the impurity accumulation is on the HFS (Cruz-Zabala *et al.* 2022) as anticipated. Impurity density variation is weak in I mode (Churchill *et al.* 2015; Cruz-Zabala *et al.* 2022), with possibly some LFS accumulation in C -Mod. Neither the radial electric field nor the electrostatic potential is a flux function based on (3.4). Moreover, the poloidal variation of the impurity density may be responsible for some of the poloidal variation of the poloidal impurity flow since $n_z V_z \cdot \nabla \vartheta / \mathbf{B} \cdot \nabla \vartheta = L_z(\psi, \vartheta)$ is not a flux function because of impurity pressure gradient terms (3.26). Then, perhaps, the assumption that the impurity flow in the pedestal is in a flux surface (Marr *et al.* 2010) is inadequate and the poloidally varying radial impurity flow, $n_z V_z \cdot \nabla \psi = -\gamma \mathbf{B} \cdot \nabla \vartheta$, is playing a role.

Finally, the large aspect ratio results reported here predict the up-down asymmetries in the impurity accumulation, but of course are unable to treat X -points and divertors as well

as strong poloidal variation. Normally the direction of the up–down asymmetry in core L mode plasmas reverses when the toroidal magnetic field reverses to change the direction of $\mathbf{B} \times \nabla B$ (Terry *et al.* 1977; Brau, Suckewer & Wong 1983; Durst 1992; Rice *et al.* 1997). Usually, the impurity accumulation is opposite to the $\mathbf{B} \times \nabla B$ direction (Brau *et al.* 1983; Rice *et al.* 1997) and does not depend on the X-point location (Rice *et al.* 1997). Additional and more relevant H mode (nominally $\eta_i < 2$) pedestal impurity asymmetry observations (Pedersen *et al.* 2002) may be broadly in agreement with Helander (1998) and Fülöp & Helander (1999, 2001) except for having asymmetries larger than predicted, occurring in pedestals with widths possibly comparable to the poloidal ion gyroradius, and perhaps not satisfying (7.4). Pedersen *et al.* (2002) also noted that observed pedestal location differences seemed consistent with a pinch velocity, possibly as expected from (7.3). Based on the simple model considered here, the $\mathbf{B} \times \nabla B$ drift is away from (toward) impurity accumulation in H mode (I mode) operation, while based on experimental observations in single null operation (Whyte *et al.* 2010; Ryter *et al.* 2017) the $\mathbf{B} \times \nabla B$ drift toward (away from) the X point is favourable for H mode (I mode). Consequently, H mode operation results in impurity accumulation away from the X point for favourable $\mathbf{B} \times \nabla B$ drift toward the X point operation. However, I mode favours accumulation toward and $\mathbf{B} \times \nabla B$ drift away from the X point.

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Declaration of interests

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Appendix A. A slightly more general solution for n

The parallel impurity momentum equation (5.24) can be solved in more detail for $1 \gg Z_i/Z_z \gg \varepsilon$ if the radial profiles are accurately known, but as they are not, perhaps it is useful to give an approximate solution to further illustrate the profile complications. Inserting n and using the exponential fits

$$\frac{\langle p_z \rangle \partial(\alpha n_c) / \partial \psi}{\alpha n_c \partial \langle p_z \rangle / \partial \psi} = -C, \tag{A1}$$

and

$$\frac{\langle p_z \rangle \partial(\alpha n_s) / \partial \psi}{\alpha n_s \partial \langle p_z \rangle / \partial \psi} = -S, \tag{A2}$$

leads to

$$(1 + \alpha)n_s = 2(G - D) + \{K + [1 + \alpha(1 - C)]D\}n_c, \tag{A3}$$

and

$$(1 + \alpha)n_c = -\{K + [1 + \alpha(1 - S)]D\}n_s. \tag{A4}$$

The solution for C and S constants is then

$$n = 1 + 2\varepsilon \frac{(G - D)[(1 + \alpha) \sin \theta - \{K + [1 + \alpha(1 - S)]D\} \cos \theta]}{(1 + \alpha)^2 + \{K + [1 + \alpha(1 - C)]D\}\{K + [1 + \alpha(1 - S)]D\}}. \tag{A5}$$

In this form the D terms are small. They give $Z_i/Z_c \ll 1$ corrections to $G \sim 1 \sim K$ that are assumed to be more important than the higher-order ε corrections that are ignored. Radial profile information is needed for the D , C and S terms as well as in G , but as the D corrections are small these terms are of limited interest other than to illustrate how non-local effects due to impurity drift departures from a flux surface enter via $\partial(\alpha n_c)/\partial\psi$ and $\partial(\alpha n_s)/\partial\psi$.

Appendix B. A solution for u in the trace limit of the banana regime

Keeping only ion-ion collisions the passing banana solubility constraint becomes

$$\left\langle \frac{B}{v_{||}} C_{ii} \left\{ h_1 - \frac{IM_i v^2 v_{||} f_{i0}}{2\Omega_i T_i^2} \frac{\partial T_i}{\partial \psi} \right\} \right\rangle = 0, \tag{B1}$$

where $\partial h_1/\partial\vartheta = 0$ and $C_{ii}\{v_{||}f_{i0}\} = 0$ in the linearized collision operator C_{ii} . For the trapped $h_1 = 0$ as the average of the drive term over a full bounce vanishes since it is odd in $v_{||}$. For $\varepsilon \ll 1$ the Kovrizhnikh model like particle collision operator (see Appendix A of Rosenbluth, Hazeltine & Hinton 1972)

$$C_{ii}\{f_{i1}\} = \frac{3\sqrt{\pi}T_i^{3/2}v_{ii}}{2M_i^{3/2}} \nabla_v \cdot \left[S(x)\nabla_v \nabla_v v \cdot \nabla_v \left(f_{i1} - \frac{M_i}{T_i} W_{||i} v_{||} f_{i0} \right) \right], \tag{B2}$$

with $x = v\sqrt{M_i/2T_i}$, $W_{||i} = 3T_i \int d^3v S v_{||} v^{-3} f_{i1} / M_i \int d^3v S v^{-1} f_{i0}$, $\text{Erf}(x) = 2\pi^{-1/2} \int_0^x dt e^{-t^2}$, $\text{Erf}'(x) = (2/\sqrt{\pi}) e^{-x^2}$ and

$$S(x) = \left(1 - \frac{1}{2x^2} \right) \text{Erf}(x) + \frac{\text{Erf}'(x)}{2x}, \tag{B3}$$

has been found to give reasonably accurate results for $\varepsilon \ll 1$. Using $\lambda = 2\mu B_0/v^2$,

$$\nabla_v \cdot (\nabla_v \nabla_v v \cdot \nabla_v f) = \frac{4B_0 v_{||}}{B v^5} \frac{\partial}{\partial \lambda} \left(\lambda v_{||} \frac{\partial f}{\partial \lambda} \right), \tag{B4}$$

leading to

$$\frac{\partial}{\partial \lambda} \left[\lambda \left\langle v_{||} \left(\frac{\partial}{\partial \lambda} \left(h_1 - \frac{IM_i v^2 v_{||} f_{i0}}{2\Omega_i T_i^2} \frac{\partial T_i}{\partial \psi} - \frac{M_i W_{||i} v_{||} f_{i0}}{T_i} \right) \right) \right\rangle \right] = 0, \tag{B5}$$

with

$$W_{||i} = \frac{3T_i \int d^3v S \frac{v_{||}}{v^3} \left(h_1 - \frac{IM_i v^2 v_{||} f_{i0}}{2\Omega_i T_i^2} \frac{\partial T_i}{\partial \psi} \right)}{M_i \int d^3v S v^{-1} f_{i0}} = \frac{3T_i \int d^3v S v_{||} v^{-3} h_1}{M_i \int d^3v S v^{-1} f_{i0}} - \frac{I[S]}{M_i \Omega_i} \frac{\partial T_i}{\partial \psi}, \tag{B6}$$

needed to conserve momentum since $C_{ii}\{v_{\parallel}f_{i0}\} = 0$, and where

$$[S] \equiv \frac{M_i \int d^3v v S f_{i0}}{2T_i \int d^3v v^{-1} S f_{i0}} = \frac{\int_0^\infty dx x^3 S(x) e^{-x^2}}{\int_0^\infty dx x S(x) e^{-x^2}}, \tag{B7}$$

with $S = 1$ giving $[1] = 1$. Integrating from $\lambda = 0$ to λ , and using $v_{\parallel}^2 = v^2(1 - \lambda B/B_0)$ to find $2v_{\parallel} \partial v_{\parallel} / \partial \lambda = -v^2 B/B_0$, leads to the passing response

$$\langle v_{\parallel} \rangle \frac{\partial h_1}{\partial \lambda} = -\frac{M_i v^2 f_{i0}}{2T_i} \left(\frac{I v^2}{2\Omega_0 T_i} \frac{\partial T_i}{\partial \psi} + \left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle \right), \tag{B8}$$

where $\Omega_0 = Z_i e B_0 / M_i c$. The ion-impurity friction and $W_{\parallel i}$ require evaluating slightly different integrals because of S . Retaining S , but noting that it is sometimes convenient to let $S \rightarrow 1$ to recover results for (5.9), and using $d^3v = dv d\lambda d\phi v^3 B_0 / v_{\parallel}$, gives (upon summing over both signs of v_{\parallel})

$$\begin{aligned} \int d^3v S \frac{v_{\parallel} h_1}{v^3} &= 4\pi \frac{B}{B_0} \int_0^\infty dv S \int_0^{1/(1+\varepsilon)} d\lambda h_1 \frac{\partial \lambda}{\partial \lambda} = -4\pi \frac{B}{B_0} \int_0^\infty dv S \int_0^{1/(1+\varepsilon)} d\lambda \frac{\partial h_1}{\partial \lambda} \\ &= \frac{4\pi M_i B}{2T_i B_0} \int_0^\infty dv v f_{i0} S \left(\frac{I v^2}{2\Omega_0 T_i} \frac{\partial T_i}{\partial \psi} + \left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle \right) \int_0^{1/(1+\varepsilon)} \frac{d\lambda}{\langle \xi \rangle}, \end{aligned} \tag{B9}$$

with $h_1 = 0$ at the trapped-passing boundary. Defining the effective passing fraction as

$$\begin{aligned} J(\varepsilon) &= \frac{B_0^2}{B^2} \int_0^{1/(1+\varepsilon)} \frac{d\lambda \lambda}{\langle \xi \rangle} / \int_0^{B_0/B} \frac{d\lambda \lambda}{\xi} = \frac{3}{4} \int_0^{1/(1+\varepsilon)} \frac{d\lambda \lambda}{\langle \xi \rangle} \\ &= \frac{3B_0}{2B} \int_0^{1/(1+\varepsilon)} \frac{d\lambda \lambda}{\langle \xi \rangle} / \int_0^{B_0/B} \frac{d\lambda}{\xi} \approx 1 - 1.46\sqrt{\varepsilon}, \end{aligned} \tag{B10}$$

the preceding becomes

$$\int d^3v S \frac{B_0 v_{\parallel} h_1}{B v^3} = \frac{M_i}{3T_i} J \int d^3v S \frac{f_{i0}}{v} \left(\frac{I v^2}{2\Omega_0 T_i} \frac{\partial T_i}{\partial \psi} + \left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle \right). \tag{B11}$$

Therefore, (B6) yields

$$\left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle + \frac{I[S]}{M_i \Omega_0} \frac{\partial T_i}{\partial \psi} = \frac{J \int d^3v S v^{-1} f_{i0} \left(\frac{I v^2}{2\Omega_0 T_i} \frac{\partial T_i}{\partial \psi} + \left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle \right)}{\int d^3v S v^{-1} f_{i0}} = J \left(\frac{I[S]}{M_i \Omega_0} \frac{\partial T_i}{\partial \psi} + \left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle \right), \tag{B12}$$

or since $J \neq 1$

$$\left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle = -\frac{I[S]}{M_i \Omega_0} \frac{\partial T_i}{\partial \psi}. \tag{B13}$$

As a result, the trace limit of (4.5) becomes

$$\begin{aligned} u &= \frac{3\sqrt{2\pi} T_i^{3/2}}{2M_i^{3/2}} \int d^3v \frac{v_{\parallel} h_1}{B v^3} = \frac{n_i}{B_0} J \left(\frac{I}{M_i \Omega_0} \frac{\partial T_i}{\partial \psi} + \left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle \right) \\ &= \frac{n_i}{B_0} J \frac{I(1 - [S])}{M_i \Omega_0} \frac{\partial T_i}{\partial \psi} \approx -\frac{0.33 J I n_i}{M_i \Omega_0 B_0} \frac{\partial T_i}{\partial \psi}, \end{aligned} \tag{B14}$$

since

$$\langle v_{\parallel} \rangle \frac{\partial h_1}{\partial \lambda} = -\frac{M_i v^2}{2T_i} \left(\frac{M_i v^2}{2T_i} - \llbracket S \rrbracket \right) \frac{I f_{i0}}{M_i \Omega_0} \frac{\partial T_i}{\partial \psi}, \quad (\text{B15})$$

where $\llbracket S \rrbracket - 1 = \{v_{ii}(x^2 - 1)\}/\{v_{ii}\} \approx 0.33$ in the notation of Fülöp & Helander (1999), and $u/I > 0$. Therefore, the constraint $K \approx G + U$ for $I > 0$ and $G > 0$ suggests $K > 0$, while for $I < 0$ and $G < 0$ it implies $K < 0$ (for $IG < 0$ the sign of K cannot be predicted). Interestingly, for $S = 1$, $u = 0 = U$, and $K \approx G$.

In addition, since $\int d^3 v f_{i0} v^2 (M_i v^2 / 2T_i - 5/2) = 0$

$$\int d^3 v v_{\parallel} h_1 = \frac{M_i B}{3T_i B_0} J \int d^3 v v^2 f_{i0} \left(\frac{I v^2}{2\Omega_0 T_i} \frac{\partial T_i}{\partial \psi} + \left\langle \frac{B}{B_0} W_{\parallel i} \right\rangle \right) = \left(\frac{5}{2} - \llbracket S \rrbracket \right) \frac{J n_i B}{M_i \Omega_0 B_0} \frac{\partial T_i}{\partial \psi}, \quad (\text{B16})$$

and

$$\int d^3 v v_{\parallel} (f_{i1} - h_1) = -\frac{I p_i}{M_i \Omega_i} \left(\frac{1}{p_i} \frac{\partial p_i}{\partial \psi} + \frac{Z_i e}{T_i} \frac{\partial \Phi}{\partial \psi} \right). \quad (\text{B17})$$

Then the parallel ion flow reduces to

$$V_{\parallel i} = \frac{1}{n_i} \int d^3 v v_{\parallel} f_{i1} = -\frac{cI}{Z_i e n_i B} \left[\left(\frac{\partial p_i}{\partial \psi} + Z_i e n_i \frac{\partial \Phi}{\partial \psi} \right) - \left(\frac{5}{2} - \llbracket S \rrbracket \right) \frac{J n_i B}{B_0} \frac{\partial T_i}{\partial \psi} \right], \quad (\text{B18})$$

where $(5/2 - \llbracket S \rrbracket) = 3/2 - 0.33 = 1.17$, as desired (Hinton & Hazeltine 1976).

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