Theoretical explanations of I-mode impurity removal and H-mode poloidal pedestal asymmetries

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Theoretical explanations of I-mode impurity removal
and H-mode poloidal pedestal asymmetries
by
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Submitted to the Department of Nuclear Science and Engineering
in partial fulfillment of the requirements for the degree of
Doctor of Science in Nuclear Science and Engineering
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Abstract

Using high-z wall materials switches the fusion challenge from heat load handling to removing impurities. I propose the first method of measuring the radial impurity flux from currently available diagnostics. It provides a means of solving the impurity accumulation problem while providing free fueling for optimum tokamak performance.

High confinement mode operation was discovered 35 years ago to almost quadruple fusion power, and later explained by turbulence reduction by sheared flows. Less than a decade ago, improved mode operation was discovered to have the same desirable property, while removing impurities and providing fueling. Thanks to the impurity radial particle flux measuring technique developed, I explain the outward radial impurity flux without invoking a (sometimes undetected) turbulent mode. This theory is supported by the observed $E \times B$ flow shear, which also explains the desired energy confinement via turbulence reduction.

Stronger impurity density in-out poloidal asymmetries than predicted by the most comprehensive neoclassical models have been measured in several tokamaks around the world during the last decade, calling into question the reduction of turbulence by sheared radial electric fields in H-mode tokamak pedestals. However, these pioneering theories neglect the impurity diamagnetic drift, or fail to retain it self-consistently as proven in this thesis, while recent measurements indicate that it can be of the same order as the ExB drift. I have developed the first self-consistent theoretical model retaining the impurity diamagnetic flow and the two-dimensional features it implies due to its associated non-negligible radial flow divergence. It successfully explains collisionally the experimental impurity density, temperature and radial electric field in-out asymmetries; thus making them consistent with H-mode pedestal turbulence reduction.

Thesis Supervisor: Peter J. Catto
Title: Senior Research Scientist
Acknowledgments

Research consists of giving birth to new ideas, that nobody has had before; sometimes they work and sometimes not, but one always acquires new knowledge on the way. The results depend not only on hard work and talent, but also on parameters out of our control. That is why I am grateful with the fact that the theoretical explanations and measuring technique proposed have turned out a success; and, hopefully, will help make the clean, safe and unlimited fusion energy available for the generations to come. This would have never happened without several people I would like to mention.

I would like to express my immeasurable gratitude to Dr. Peter Catto for teaching me by example how to be an outstanding supervisor, researcher and person. Thank you for both everything you have taught me and especially for always believing in me. I cannot thank you enough for all the time you spent during my first semester patiently challenging me at the blackboard with turbulence and transport problems, being such an inspiration for me to do that for other students one day. Thank you also for letting me take afterwards way more responsibility and leadership than normally allowed so I could develop as a researcher humbly following your example, having corrected the literature and even proposed novel research topics for publication.

I would also like to extend my gratitude to the committee members Prof. Ian Hutchinson, Prof. Jeff Freidberg and Prof. Dennis Whyte for transmitting their knowledge, brilliant teaching skills, research experience, motivation and humanity. Thank you for having been an intellectual stimuli, by encouraging the quality, the analysis capacity and, specially, going further in understanding the mathematical, physical and numerical concepts. Moreover, I would also like to acknowledge Prof. Ian Hutchinson’s constructive criticism, advise and editing efforts to improve the presentation in this thesis. I am grateful to all of the teachers, researchers, other members of the staff, classmates, labmates, universitymates and housemates, which become friends, for their invaluable insight, help and support in and out of class.

Back to my roots, infinite thanks to Prof. Ignacio Romero, I still cannot believe
how lucky I have been of having meet you, thank you so much for introducing me to the research activity and specially for transmitting me your passion for doing research.

Special thanks to my life-long friends, particularly to Elena; and to each one of my family, specially to my parents Jesús Manuel and Inmaculada, my sister Irene and my boyfriend Nathaniel, for making me who I am in all aspects. Thank you for being always there, for all the sacrifices that you have made so I could put so much effort into this thesis, for your unconditional support and love. This thesis is yours. I love you. Finally, thank You, for making possible for this to be just the beginning.
Patents, publications, awards and invited talks

• Patents

The first method of measuring the radial impurity flux proposed in this thesis is being patented under U.S. Application No.: 62/476930.

• Publications

The ideas, theoretical models and results described in this thesis are inspiring the improvement of fusion codes and further experiments to further test the model predictions. Most importantly, it also suggests optimum tokamak designs to actively prevent impurity accumulation. Each of the chapters of the thesis corresponds to the following publications:


• **Awards**

I am indebted to the following national and international awards, recognition and support that this research project have received:

- 2017: ‘Rafael del Pino’ highly-selective postdoctoral Fellowship (<3% acceptance rate).

- 2016: International Sherwood Fusion Theory Award for excellent graduate student presentation.

- 2016: European Physics Society EPS/PPCF/IUPAP Student Poster Prize.

- 2014: Alpha Nu Sigma Award to top academic performances.

- 2013: ‘La Caixa’ highly-selective doctoral Fellowship (<5% acceptance rate).

• **Invited talks**

I am also grateful for having been selected to give the following invited talks:


A mi familia y a Nathaniel
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Silvia Espinosa Gútiez (sesp@mit.edu) 21/ 214
# Introduction and motivation

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1.1 The fusion challenge of impurity avoidance and removal and energy confinement

1.1.1 Fusion challenge: heat handling to impurity removal

The Sun is an illustrative example of a plasma that provides fusion energy to our planet, providing us with light and heat every single day. The aim of the international fusion research is creating a mini-Sun on Earth. The solar flares shown in Fig. 1.1 makes it easy to understand that fusion used to be challenged by finding materials that will not melt even when put extremely close to the surface of the Sun.

The usage of high-z wall materials switches the fusion challenge from heat load handling to removing the associated impurities [8]. Tokamaks are currently challenged by the large radiative energy losses produced when highly charged di-

Figure 1.1: Sun erupting solar flares overlapped by a tokamak cross section with metal walls and divertor.
Impurities are absorbed through the pedestal and accumulate in the core of the plasma \cite{9} (Fig. 1.2(a)). The radiative energy losses produced by these impurities can compromise tokamak performance in the JET ITER-like wall (JET-ILW) \cite{10,12} and ASDEX-Upgrade \cite{13} experiments, that mimic the ITER tungsten divertor, and in Alcator C-Mod with its molybdenum divertor \cite{14}.

Fusion performance can be substantially improved by reducing the inward radial impurity flux and, even better, changing its sign such that impurities are naturally pumped out of the plasma core (Fig. 1.2(b)). To preserve ambipolarity \cite{15}, when only a single impurity species is present, theory indicates that the background ions that fuel the plasma must go inward when the impurity species goes outward, as electron transport is weak.

In this thesis I propose a method of measuring the radial impurity flux \cite{2,3}...
CHAPTER 1. INTRODUCTION AND MOTIVATION

Figure 1.3: Confinement mode characteristics with respect to impurity and energy confinement and I-mode pioneering identification criterion.

from currently available diagnostics [16]. The discovery of its driving forces is used to provide insight into the optimal tokamak operation to actively solve the impurity accumulation problem, while providing free fueling for optimum tokamak performance.

1.1.2 Theoretical explanation of I-mode impurity removal

High confinement mode (H-mode) operation was discovered 35 years ago [17] to almost quadruple fusion power with respect to the low confinement mode (L-mode), and later explained by turbulence reduction by sheared flows [18]. Less than a decade ago, improved mode operation (I-mode) was discovered [19] to have the same desirable property, while removing impurities and providing fueling. I-mode is not only a possible breakthrough solution to the core high charge number impurity accumulation challenge, but it also may successfully prevent plasma dilution by eliminating ash from the core.

The two ideal properties in a confinement mode, energy confinement and impurity removal, are represented in the axis in Fig. 1.3. While H and L-mode present
the former and latter respectively, I-mode is the most favorable by exhibiting both, as indicated by its location on the upper right corner. The presence of a weakly coherent oscillation in I-mode, as shown in Fig. 1.4 was originally proposed \cite{19} as a method to distinguish it from the H-mode. Nonetheless, modes exhibiting the same characteristics as an I-mode with high energy confinement and low particle confinement but without the detection of the weakly coherent mode have been observed, perhaps due to its extreme spatial localization.

Thanks to the impurity radial particle flux measuring technique developed, I offer an alternative explanation of the outward radial impurity flux without invoking a (sometimes undetected) turbulent mode. This explanation is consistent with the observed $\mathbf{E} \times \mathbf{B}$ flow shear in both I mode and H mode, which may explain the desired improved energy confinement via turbulence reduction. I also propose a criterion to distinguish I-mode from H-mode.

1.1.3 Theoretical explanation of H-mode pedestal turbulence reduction

It has been suggested \cite{21,22} that the sudden transition between states of low (L) and high (H) confinement, the L-H transition, involves the reduction of turbulence by the strongly sheared radial electric field in the pedestal. For H-mode pedestals,
the amplitudes of the turbulence may be only large enough to affect higher order phenomena in a poloidal gyroradius expansion, such as heat transport. Neoclassical collisional theory may then be expected to and is normally assumed \[15,23,27\] to properly treat lower order phenomena, such as flows.

Stronger impurity density in-out poloidal asymmetries than predicted by the most comprehensive neoclassical models have been measured in several tokamaks around the world during the last decade \[20,28,32\] as illustrated in Fig. 1.5, calling into question the applicability of neoclassical impurity transport in H-mode tokamak pedestals \[20\].

However, these pioneering theories \[2,3,15,23,27\] neglect the impurity diamagnetic drift, or fail to retain it self-consistently \[33\] as proven in this thesis, while
recent measurements indicate that it can be of the same order as the ExB drift.

In this thesis I have developed the first self-consistent theoretical model retaining the impurity diamagnetic flow and the two-dimensional features it implies due to its associated non-negligible radial flow divergence. It can obtain collisionally the experimental values of impurity density, temperature and radial electric field in-out asymmetries simultaneously for physical values of the impurity diamagnetic flow; thus making them consistent with H-mode pedestal turbulence reduction.

1.2 Neoclassical theory of impurity transport

An impure tokamak edge is often modeled by allowing the flows to be large enough that the friction of the collisional highly-charged impurity species with the banana, Pfirsch-Schlüter or plateau main ions competes with the parallel impurity pressure gradient and parallel electric field. In contrast to the flows are often assumed smaller than the impurity thermal velocity in order to self-consistently neglect the inertial force.

The Pfirsch-Schlüter flows arise to ensure that the divergence of the current vanishes, which the diamagnetic current cannot guarantee on its own in the toroidal geometry characteristic of a tokamak. The collisionality regime of the background ions determines the sign of the ‘temperature screening’ in the background ion flow, proportional to the radial gradient of the bulk ion temperature. For trace impurities, the ‘temperature screening’ in the parallel impurity flow in the direction of the magnetic field for the plateau and Pfirsch-Schlüter regimes, being smaller and larger respectively. In contrast, it has the opposite direction than the magnetic field in the banana regime. The presence of a significant amount of impurities and poloidal variation could affect these results.

The parallel friction is related to the flux-surface-averaged radial impurity flux, by employing conservation of toroidal momentum for the impurities.
For the low flow ordering, the poloidal electric field rearranges the impurities poloidally on a pedestal flux surface to minimize the parallel friction with the background ions and thereby allow inboard impurity accumulation [15].

During the last two decades, the state-of-the-art neoclassical pedestal theories for impurity behavior [15,23,25,35] have been analyzing the impurity parallel dynamics independently. In other words, the physical phenomena included were cleverly selected [15] such that the interesting effects of the impurity radial flow could be self-consistently neglected for simplicity when evaluating its parallel flow and treating conservation equations:

- First, the highly-charged collisional impurity is allowed to be non-trace, i.e. its density is taken to be large enough to affect the bulk ion dynamics by allowing the collisional frequency of bulk ions with impurities to compete with the self-collision frequency of the background.

- Second, the impurity and main ion flows are assumed significantly weaker than the thermal velocity of the impurities, since the characteristic perpendicular length scales are much larger than the impurity poloidal gyroradius.

- Third, the impurities are taken to be in thermal equilibrium with weakly poloidally varying background ions. The bulk ion temperature is taken to be a lowest order flux function in order to self-consistently assume Maxwell-Boltzmann bulk ion response. This is justified by the fact that the observed temperature variation [20] is substantially weaker than that of the impurity density. The poloidal variation in the impurity temperature could be driven by other terms in the energy equation.

- Fourth, the key simplifying assumptions towards neglecting the impurity radial flows rely on taking the pedestal characteristic length to be of the same order for both impurity and main ion densities and on taking the charge number of the impurities very large. In this way the diamagnetic
flow can be neglected for high charge state impurities, while it is retained for the bulk ions. As a result, the impurity parallel momentum equation only need retain parallel pressure and electric field terms to balance the parallel friction with the background ions.

1.3 Successes and failures of neoclassical theory to explain experiments

These existing theories continue to provide valuable insight into the poloidal rearrangement within a flux function of impurities in thermal equilibrium with weakly poloidally varying background ions. The primary reason being that Helander [15] proved that impurities can accumulate on the inboard side of a flux surface due to the friction with the background ions. His model allows the friction to compete with the potential and pressure gradient terms in the impurity parallel momentum conservation equation. The drive for this impurity density in-out asymmetry is given by the poloidal variation of the magnetic field. The inverse dependence of the bulk diamagnetic flow on the magnetic field magnitude can cause the impurity density to be higher on the high field side than on the low field side. If the impurity toroidal rotation was large enough, the inertial term should be retained and the centrifugal force could then compete with or overtake the previous phenomena, causing the highly-charged impurities to concentrate on the low field side [25].

The original model with banana regime main ions [15] was extended to the Pfirsch-Schlüter [23] and plateau [24] collisionality regimes, in the hope of obtaining larger impurity concentration on the high field side. However, high confinement mode edge pedestals on Alcator C-Mod [20,28,29] exhibit somewhat stronger poloidal variation than predicted by the most comprehensive neoclassical theoretical models developed to date [15,23,24,35], indicating that there may be
some physical process missing from these models. This missing phenomenon may
further amplify the magnetic field in-out asymmetry, which is the only drive in
previous theories, or perhaps act as an additional drive. Impurity peaking at the
inboard side is also observed in other tokamaks, such as ASDEX-U \[30,31\] and
JET \[32\]. In addition, up-down asymmetries have also been detected on toka-
maks, such as Alcator A \[36\], PLT \[37\], PDX \[38\], ASDEX \[39\], Compass-C \[40\]
and Alcator C-Mod \[41–43\].

In this thesis I propose a self-consistent two-dimensional theoretical neoclassi-
cal model for axisymmetric tokamak pedestals. In contrast to the previous one-
dimensional models \[15,23–25,35\], the impurity parallel dynamics is affected not
only by flows contained in the flux surface but also by the impurity radial flows
out of the flux surface. The novel expressions for the impurity flow and conserva-
tion equations improve our ability to model pedestals and perhaps extend existing
codes \[44,45\] to a new dimension. More importantly, this pedestal neoclassical
model with radial flows may ultimately suggest how to better control or even avoid
impurity accumulation in tokamaks such as JET and ASDEX-Upgrade.

Radial flow effects become important when the impurity density exhibits very
strong radial gradients. We achieve self-consistency by allowing the impurity dia-
magnetic drift to compete with the $\mathbf{E} \times \mathbf{B}$ drift, as supported by experimental
observations \[29\]. Radial and diamagnetic flow effects substantially alter the par-
allel impurity flow. The resulting modification in the impurity friction with the
banana regime background ions impacts the impurity density poloidal variation,
by acting as an amplification factor on the magnetic field poloidal variation drive.
It can lead to stronger poloidal variation that is in better agreement with the ob-
servations for physical values of the diamagnetic term. In addition, the poloidally-
dependent component of the radial electric field can compete with its flux surface
average for the first time, introducing poloidal variation not contained in previous
models. Finally, compressional heating now prevents complete equilibration be-
tween impurities and the main ions, resulting in an impurity temperature in-out asymmetry.

1.4 Thesis problems addressed and structure of the thesis

The thesis structure is summarized in Table A.1 and consists of two main parts. This table also contains the publications corresponding to each chapter.

1.4.1 Part I: Pedestal radial flux measuring method and theoretical explanation of I-mode impurity removal

The first part proposes a radial impurity flux measuring technique from available diagnostics. Devising a means to measure the radial impurity flux across the pedestal could be used to reduce impurity accumulation, if not prevent it while providing natural fueling, and thus improving fusion performance in tokamaks.

Chapter 2 illustrates in the large aspect ratio limit the novel solution procedure that takes advantage of the poloidal flow measurement to obtain the radial impurity flux directly from available diagnostics, such as charge exchange recombination spectroscopy and Thomson scattering, without the need of a computationally demanding kinetic calculation of the full bulk ion response. It suggests how to actively optimize tokamak operation and favourably modify the profiles to prevent impurity accumulation.

Chapter 3 systematizes and generalizes the measuring method to allow for larger flows, plasma heating and seeding for general tokamak cross sections. This extension is motivated in part by the fact that ion cyclotron resonance heating of minority ions and toroidal rotation can be used to actively and favorably modify the poloidal variation of the potential to adjust the location of impurity accumu-
lation and thereby alter the radial impurity flux.

Chapter 4 uses the measuring technique to show that outward collisional radial impurity flux seems to be a robust distinguishing characteristic between I-mode and H-mode, rather than the turbulent weakly coherent mode that is sometimes undetected, perhaps due to its strong spatial localization. In both I and H regimes the \( \mathbf{E} \times \mathbf{B} \) flow shear observed may break up eddies to reduce the turbulence level, leading to good bulk energy confinement.

This measuring method implies a new technique of solving the equations that can be applied to any neoclassical model. For illustrative purposes, the impure tokamak edge is modeled by allowing the parallel dynamics to be studied independently, in a one-dimensional fashion, in the first part of the thesis. This model \cite{espinosa2015} is adequate for very high-z impurities, such as tungsten or molybdenum.

Part II of this thesis presents a more general derivation of this equation by retaining impurity diamagnetic and radial flow effects. This model, targeted for not so highly charged impurities such as boron or carbon, properly reduces to the one-dimensional model used in the first part of the thesis when the diamagnetic and radial effects are ignored. The reader who wants more details of the model used in the first part of the thesis is referred to the second part of the thesis for a detailed derivation.

1.4.2 Part II: Theoretical explanation of pedestal poloidal variation, addressing the concern regarding H-mode pedestal turbulence reduction

The second part of the thesis, starting with Chapter 5, presents a self-consistent non-linear theoretical model retaining the impurity diamagnetic flow and the two-dimensional features it implies due to its associated non-negligible radial flow divergence. It demonstrates that the previous literature \cite{espinosa2015} claiming to include diamagnetic effects one-dimensionally is flawed. The model, targeted for not so
highly charged impurities such as boron or carbon, properly reduces to the one-dimensional model when the diamagnetic and radial effects are ignored.

Chapter 6 solves the linear and non-linear forms of the parallel momentum equation to demonstrate the model’s ability to capture the experimental features and values of impurity density in-out asymmetry.

Chapter 7 addresses the energy equation of the neoclassical model with impurity temperature poloidal variation. It is driven by the compressional heating in the energy equation, which prevents the complete equilibration of impurity and bulk ion temperatures, assumed in previous theories. The impurity density and temperature in-out asymmetry are simultaneously captured and a sharp prediction of the pedestal profile alignment to be used is provided.

Finally, Chapter 8 presents the conclusions drawn from both parts of this research project.
Part I

Pedestal radial flux measuring method and theoretical explanation of I-mode impurity removal

(1D: Chap. 2 - 4)
Chapter 2

Pedestal radial flux measuring method to prevent impurity accumulation


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2.1 Introduction

Tokamaks are currently challenged by the large radiative energy losses produced when highly charged divertor impurities are absorbed through the pedestal and accumulate in the core of the plasma [9] (Fig. 1.2(a)). This can compromise tokamak performance in JET ITER-like wall (JET-ILW) [10–12] and ASDEX-Upgrade [13], that mimic the ITER tungsten divertor, and in Alcator C-Mod with its molybdenum divertors [14].

Fusion performance can be substantially improved by reducing the inward radial impurity flux and, even better, changing its sign such that impurities are naturally pumped out of the plasma core (Fig. 1.2(b)). To preserve ambipolarity [15], theory indicates that, accounting only for collisional momentum exchange of the background ions with a single impurity species, the ions and impurities are transported in opposite directions. Determining how to measure radial impurity flux across the pedestal and discovering its driving forces could thus assist with optimizing tokamak operation to prevent impurity accumulation while providing natural fueling.

It has been suggested [21,22] that the sudden transition between states of low (L) and high (H) confinement, the L-H transition, involves the reduction of turbulence by the strongly sheared radial electric field in the pedestal. For H-mode pedestals, the amplitudes of the turbulence may be only large enough to affect higher order phenomena in a poloidal gyroradius expansion, such as heat transport. Neoclassical collisional theory may then be expected to and is normally assumed [15,23–27] to properly treat lower order phenomena, such as flows.

Specifically, an impure tokamak edge is often modeled [15] by allowing the flows to be large enough that the friction of the collisionally highly-charged impurity species with the banana [15], Pfirsch-Schlüter [23] or plateau [24] main ions competes with the parallel impurity pressure gradient and parallel electric field.
In contrast to [25–27], the flows are assumed smaller than the impurity thermal velocity in order to self-consistently neglect the inertial force.

The parallel friction is related to the flux-surface-averaged radial impurity flux [15], by employing conservation of toroidal momentum for the impurities. For the low flow ordering, the poloidal electric field rearranges the impurities poloidally on a pedestal flux surface to minimize the parallel friction with the background ions and thereby allow inboard impurity accumulation [15].

Impurity peaking on the inboard side is observed in tokamaks such as Alcator C-Mod [20,28,29], ASDEX-U [30,31] and JET [32]. In addition, up-down asymmetries have also been detected on tokamaks such as Alcator A [36], Princeton Large Torus (PLT) [37], Poloidal Divertor Experiment (PDX) [38], ASDEX [39], Compass-C [40] and Alcator C-Mod [41–43].

Charge-exchange recombination spectroscopy [16,30,46] is used to measure the low (LFS) and high field side (HFS) boron density, temperature and importantly poloidal and toroidal mean flow radial profiles in the midplane pedestal region of Alcator C-Mod and ASDEX-U (Fig. 2.1(a)).

In general, a calculation of the impurity radial flux requires solving the main ion kinetic equation. Insightful solutions have been obtained at large aspect ratio for trace impurities or when impurity-ion collisions dominate over ion-ion collisions [25]. However, a numerical approach is needed in realistic situations with non-trace impurities having strong poloidal variation.

Here we illustrate how available diagnostics can be used to bypass the computationally demanding calculation of these kinetic effects by expressing them in terms of the poloidal flow. In Sec. 2.2 we first show how the radial impurity flux in the pedestal can be re-expressed as a sum of two terms involving only the poloidal mean flow, the impurity density in-out asymmetry and the main ion radial density and temperature profiles. We then show how this form provides a precise means of calculating the neoclassical radial flux for non-trace impuri-
CHAPTER 2. PEDESTAL RADIAL FLUX MEASURING METHOD

Figure 2.1: Diagnostics proposed to measure the radial impurity flow directly from available measurements.

2.2 Deriving local impurity radial flow from local diagnostics

In this section, the main ion kinetic effects are related to the poloidal impurity flow. This allows us to express the neoclassical radial impurity flux as a function of
measurements already available via charge-exchange recombination spectroscopy and Thomson scattering.

2.2.1 Sign convention

The axisymmetric tokamak magnetic field is given by $\mathbf{B} = I \nabla \zeta + \nabla \zeta \times \nabla \psi$; where $I = R B_t$, with $R$ the major radius and $B_t$ the toroidal (subscript $t$) magnetic field. The poloidal ($p$) magnetic field is given by $R B_p = |\nabla \psi|$, with $2\pi \psi$ the poloidal magnetic flux.

The direction of the poloidal and toroidal angles, denoted by $\theta$ and $\zeta$ respectively, is chosen such that $\mathbf{B} \cdot \nabla \theta$ and the flux function $I$ are positive. Moreover, the components of the mean flow $\mathbf{V}$ are considered positive when in the direction of the magnetic field. This sign convention is illustrated on a schematic tokamak cross-section in Fig. 2.2, and compared to that of Alcator C-Mod experiments [29] (Fig. 2.2(a)). While the sign convention adopted for the flows is the same as the C-Mod experimental one for normal or forward field operation (Fig. 2.2(b)), it is the opposite when the magnetic fields are reversed (Fig. 2.2(c)).
2.2.2 Impurity-main ion friction

The plasma is taken to be composed of Maxwell-Boltzmann banana regime electrons and bulk ions \( i \) with charge number \( z_i \sim 1 \), together with a highly-charged collisional impurity \( z \) whose density \( n_z \) satisfies \( z_z^2 n_z \lesssim z_i^2 n_i \). Although the impurity does not significantly alter the lowest-order quasineutrality, its density is large enough to affect the bulk ion dynamics by allowing main ion self-collisions and collisions with impurities to compete. Under these assumptions, the friction force exerted on the impurities by the bulk ions in the direction parallel (\( \parallel \)) to the magnetic field is \[ F_{z\parallel} = \frac{M_i \langle n_z \rangle}{n_z} \nu_{iz} \left[ \frac{cI \langle p_i \rangle}{z_i e} \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) \left( \frac{B^2}{\langle B^2 \rangle} - \frac{n_z}{\langle n_z \rangle} \right) \right. 
\]

\[ + u B^2 \left( \frac{n_z}{\langle n_z \rangle} - \left( \frac{B^2}{\langle B^2 \rangle} \frac{n_z}{\langle n_z \rangle} \right) \right) \] (2.1)
for arbitrary aspect ratio; where \( c \) and \( e \) are the speed of light and the magnitude of the electron charge. Each of the species has mass \( M \) and pressure \( p = nT \), with \( T \) denoting the temperature. The reader is referred for details to Chapter 5.3, where (2.1) can be recovered by substituting into (5.29) the first line of (5.56), since the second one contains impurity diamagnetic and radial flow effects that are only included in Part II.

The flux surface average of a quantity \( Q \) is defined as
\[ \langle Q \rangle = \frac{\oint Q d\theta}{\oint d\theta} = \frac{\oint Q d\theta}{2\pi} ; \]
where \( \vartheta \) is a modified poloidal angle coordinate, satisfying \( \frac{d\theta}{B \nabla \vartheta} = \frac{d\vartheta}{B \nabla \theta} \). The collision frequency of impurities with bulk ions divided by the impurity density, \[ \nu_{iz} = \frac{4\sqrt{2\pi} z_i^2 z_z^2 e^4 \ln \Lambda}{3M_i^2 T_i^2} , \] (2.2)
is a flux function; since the Coulomb logarithm \( \ln \Lambda \) and the bulk ion temperature are taken to be flux functions. Moreover, the following integral over bulk ion velocity space \( v \),
\[ u = \frac{3\sqrt{\pi}}{\sqrt{2}} \frac{T_i^3}{M_i^3} \int \frac{d^3v}{B} \frac{v_i}{v^3} h_i, \tag{2.3} \]

is also a flux function for banana main ions \[15\]. Here the bulk ion kinetic response \( h_i \) is related to the gyroaveraged first-order main ion distribution function and vanishes in the trapped domain, but an explicit evaluation is not required. Indeed, one of the main purposes of this paper is to avoid the need to numerically solve the bulk ion kinetic equation to evaluate \( h_i \).

The background ion kinetic response \( h_i = f_i - f_{iM}^*(\psi^*_i, E_i) \) vanishes in the trapped domain, where \( f_i \) is the main ion distribution function. The distribution \( f_{iM}^* \) is a modification of a Maxwell-Boltzmann distribution depending only on the constants of the motion canonical angular momentum \( \psi^*_i = \psi - \frac{z_i e}{M_i c} R^2 \nabla \zeta \cdot \mathbf{v}_i \), which replaces the \( \psi_i \) dependence, and total energy \( E_i = \frac{v_i^2}{2} + \frac{z_i e \Phi}{M_i} \). The algebraic details regarding the calculation of \( h_i \) are also relegated to Appendix C.

### 2.2.3 Obtaining the radial impurity flux from available diagnostics

The radial component of the impurity particle flux, \( \Gamma_z = n_z V_z \), is related to the parallel friction \[2.1\] by using the toroidal projection of the conservation of impurity parallel momentum equation \[15\]. Insight on a novel technique to measure the radial impurity flux is obtained by Taylor expanding the flux surface averaged impurity radial flux for small inverse aspect ratio, \( \epsilon \ll 1 \), and using the solubility constraint that corresponds to the conservation of canonical angular momentum, \( \langle BF_{z||} \rangle = 0 \), to find:

\[
\frac{\langle \mathbf{T}_z \cdot \nabla \psi \rangle}{\frac{\epsilon}{z_i e (B^2)}} = -\langle B^2 \rangle \left\langle \frac{F_{z||}}{B} \right\rangle = \left\langle \frac{-BF_{z||}}{1 + (b^2 - 1)} \right\rangle = \langle BF_{z||} (b^2 - 1) \rangle \left[ 1 + O(\epsilon) \right]. \tag{2.4} \]
CHAPTER 2. PEDESTAL RADIAL FLUX MEASURING METHOD

Here both the poloidal variation of the square of the dimensionless magnetic field, $b^2 = \frac{B^2}{\langle B^2 \rangle}$, and the impurity density, $n = \frac{n_z}{\langle n_z \rangle}$, are retained.

Substituting the parallel friction (2.1) into (2.4), noticing that $b^2 (n - \langle b^2 n \rangle) = (n - 1) [1 + O(\epsilon)]$, the radial impurity flux can be conveniently expressed in terms of flux functions to second-order accuracy as

$$\langle \Gamma_z \cdot \nabla \psi \rangle = \langle n - 1 \rangle \left( b^2 - 1 \right) \left( g + U \right) - \left( 1 - b^2 \right)^2 g; \quad (2.5)$$

where, apart from the large aspect ratio expansion, only $n - 1 \ll 1$ is required to neglect higher order corrections. Consequently, the impurity density could in principle have a stronger poloidal variation than the magnetic field, for instance, of order $\sqrt{\epsilon}$. The dimensionless coefficients

$$g = - \frac{c I}{z_e e \langle B \cdot \nabla \theta \rangle} \frac{M_i}{n_z} \frac{T_z}{\langle T \rangle} \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) \quad (2.6)$$

and

$$U = \frac{u \langle B^2 \rangle}{\langle T \rangle} \frac{M_i}{\langle B \cdot \nabla \theta \rangle} \frac{\nu_{iz}}{n_z} \quad (2.7)$$

indicate the contributions of the fluid and kinetic bulk ion responses, respectively. Here, $g \sim U \sim \frac{qR}{\lambda_z \rho_{pi} L_i}$, with $qR$ the connection length and $\lambda_z$ the impurity mean free path taking into account both like and unlike collisions. The main ion poloidal Larmor radius and characteristic radial scale length are denoted by $\rho_{pi}$ and $L_i$.

Charge-exchange recombination spectroscopy is used to measure the outboard (LFS) and inboard (HFS) impurity temperature, density, and poloidal and parallel mean flow radial profiles for intrinsic impurities up to argon (e.g. boron and carbon). The experimental challenges posed by the multiple charge states exhibited by some highly-charged impurities (e.g. molybdenum and tungsten) may possibly be overcome by using bolometric, ultraviolet, soft X-rays, or perhaps even on X-ray crystal spectrometer with poloidal views, as used for different argon charge states [48]. In addition, the main ion temperature and density can be estimated by the impurity temperature and electron density as measured by
CHAPTER 2. PEDESTAL RADIAL FLUX MEASURING METHOD

charge-exchange recombination spectroscopy and Thomson scattering respectively, due to ion-impurity temperature equilibration and quasineutrality [2].

For illustrative purposes, a first-order cosinusoidal profile is considered for the known dimensionless magnetic field, $b^2 = 1 - 2\epsilon \cos \vartheta$; and a first-order Fourier profile for the dimensionless impurity density, with both a sinusoidal and a cosinusoidal term in order to allow for up-down and in-out asymmetries respectively. Only the measured impurity density in-out asymmetry term contributes to the following flux surface average needed to calculate the radial impurity flow (2.5),

$$\langle (n - 1) (b^2 - 1) \rangle = \epsilon \frac{n_{HFS} - n_{LFS}}{n_{HFS} + n_{LFS}},$$  

(2.8)

which is positive for inboard impurity accumulation. For this angular variation and trace impurities, it can be deduced from Sec. IV.A in [25] that there is inboard accumulation when $g$ and $g+U$ have the same sign for low flows. As a consequence, the two terms of the radial impurity flux in (2.5) have opposite signs.

The same conclusion is drawn for very large gradients, i.e. friction dominating the parallel momentum equation. In this case, taking the large aspect ratio limit of Eq. (11) in [15] gives $\frac{g}{g+U} = \frac{g}{g+U}$. The results in this paper allow the impurity density poloidal variation to be larger than that of the magnetic field if $g+U \ll g$, although they are also valid when $g + U \sim g$.

Importantly, the impurity poloidal mean flow in [15], which can be measured by charge-exchange spectroscopy, can be used to obtain $g + U$ in (2.5) to lowest order by noticing that

$$\frac{n_z V_z \cdot \nabla \theta}{B \cdot \nabla \theta} = -\frac{eIT_i}{z_i e} \langle n_z \rangle \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) + u \langle B^2 n_z \rangle \langle B^2 \rangle \langle n_i \rangle$$

(2.9)

where we use $\langle b^2 n \rangle = 1 + O[\epsilon (n - 1)]$. It can thus be observed that when $g + U$ is positive the poloidal impurity flow goes in the direction of the poloidal magnetic field.
Next, the radial gradient of the main ion density appearing in $g$ in Eq. (2.6) can be obtained from Thomson scattering measurements of the radial pedestal electron density profile, by using lowest order quasineutrality, $z_i \langle n_i \rangle = \langle n_e \rangle$. The electron temperature is also available via Thomson scattering, while the impurity temperature is known from charge-exchange spectroscopy. Although all the temperatures are typically of the same order, it is better to use the impurity (rather than the electron) temperature to estimate the bulk ion temperature due to the more rapid ion-impurity energy equilibration. Note that $g$ is negative if the descending slope of the logarithmic temperature is more than twice as steep as that of the logarithmic density for main ions, $\frac{d \ln T_i}{d \ln \langle n_i \rangle} > 2$, and positive otherwise.

### 2.3 Suggested tokamak operation to avoid impurity accumulation

The proposed method allows not only the measurement of the radial impurity flux but also provides insight into the favourable physical phenomena preventing impurity accumulation while achieving natural fueling. A detailed analysis of the profile characteristics that allow us identify optimal tokamak operation ‘a posteriori’ is provided in this section, together with illustrative examples of its usage. Suggestions on promising experimental procedures to favorably modify each term of the radial flux are discussed separately. Hopefully, these ideas will lead to further measurements on the effectiveness of these techniques on minimizing the inward radial impurity flux term while maximizing the outward one.

#### 2.3.1 Impurity poloidal flow and density in-out asymmetry

The direction of the first component of the neoclassical pedestal radial impurity flux in (2.5) depends on both the impurity poloidal flow direction (2.9) and density
CHAPTER 2. PEDESTAL RADIAL FLUX MEASURING METHOD

Table 2.1: Direction of the first neoclassical pedestal radial impurity flux component in (2.5), as a function of the impurity poloidal flow direction and density in-out asymmetry obtainable by charge-exchange spectroscopy.

<table>
<thead>
<tr>
<th>Poloidal impurity flow and magnetic field directions</th>
<th>Impurity accumulation</th>
<th>HFS</th>
<th>LFS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co $(g+U &gt; 0)$</td>
<td>Out</td>
<td></td>
<td>In</td>
</tr>
<tr>
<td>Counter $(g+U &lt; 0)$</td>
<td>In</td>
<td>Out</td>
<td></td>
</tr>
</tbody>
</table>

in-out asymmetry (2.8). As explained in Table 2.1, it removes impurities from the plasma core while absorbing fuel in the following two cases:

- The poloidal flow is in the direction of the magnetic field and there is HFS impurity accumulation.
- The poloidal flow and magnetic field are in opposite directions and there is LFS impurity accumulation.

Impurity poloidal flow in the direction of the magnetic field and HFS impurity accumulation have been observed in both ASDEX-U [31] and Alcator C-Mod [49] for different types of H-modes: Enhanced D-Alpha (EDA) at lower (Fig. 4.4 in [49]) and higher safety factor (Fig. 4.5), Edge-Localized Mode(ELM)-free (Fig. 4.6) and ELMy (Fig. 4.7). These measurements, with $\mathbf{B} \times \nabla B$ towards the X-point, indicate a favorable outward neoclassical radial impurity flux for the first term.

Even though the physics included in the model has been limited here to illustrate how to infer radial fluxes from charge exchange and Thomson data, it is worth pointing out that there are practical methods of modifying tokamak in-out asymmetry such as neutral beam driven rotation or plasma heating. The centrifugal force associated with the toroidal rotation has been proven to push impurities outwards towards the LFS of each flux surface [25]. In contrast, neutral beam injection or ion cyclotron resonance heating (ICRH) of minority ions provide a
CHAPTER 2. PEDESTAL RADIAL FLUX MEASURING METHOD

\[ \frac{d\ln T_i}{d\ln n_e} \quad g \quad (2.6) \quad \text{Direction of 2}^{nd} \text{ impurity radial flux term (2.5)} \]

<table>
<thead>
<tr>
<th>( \frac{d\ln T_i}{d\ln n_e} )</th>
<th>( g )</th>
<th>Direction of 2(^{nd} ) impurity radial flux term (2.5)</th>
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<tbody>
<tr>
<td>&lt; 2</td>
<td>+</td>
<td>In</td>
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<tr>
<td>&gt; 2</td>
<td>-</td>
<td>Out</td>
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**Table 2.2:** Direction of the second neoclassical pedestal radial impurity flux component in (2.5), as a function of the ratio of main ion temperature to density gradients.

mechanism for HFS impurity localization. Fast ions produced by neutral beam injection or ion cyclotron resonance heating of minority ions tend to concentrate on the outboard side. Quasi-neutrality then forces the highly charged impurities towards the HFS [27].

2.3.2 Main ion radial density and temperature profiles

The direction of the second neoclassical pedestal radial impurity flux component in (2.5) is determined by the radial profiles of the main ion temperature and density. As explained in Table 2.2 it pumps out impurities when the background ion temperature is more than twice as steep as the density.

The appropriate tokamak operation can be identified by using a logarithmic plot of electron density gradient scale-length versus electron (or better yet, impurity, if available) temperature gradient scale-length. This is illustrated by Fig. 13 of [19] (Fig. 2.3), where only the 20% of plotted EDA and the 50% of ELM-free H-modes, with \( \mathbf{B} \times \nabla \mathbf{B} \) towards and away from the X-point respectfully, are located in the region with \( \eta = \frac{d\ln T_e}{d\ln n_e} > 2 \). Those discharges exhibit favourable outward second term of the neoclassical radial impurity flux and are expected to prevent impurity accumulation while providing natural fueling.

There are several experimental techniques to affect the relative slope of the radial electron density and temperature profiles; such as fueling, mode excitation, recycling and impurity seeding. On the one hand, a high density region driven
Figure 2.3: Electron temperature gradient scale-length versus density gradient scale-length evaluated at the symmetry location of the Te pedestal (Fig. 13 of [19]).

by gas puffing and heating power has been observed in the high field side scrape-of-layer at JET [50] and ASDEX-Upgrade [51]. In these cases the scrape-of-layer density is around ten times larger than at the separatrix and the dominant plasma fueling mechanism is diffusive neutral penetration. This effectively alters the electron pedestal profiles by shifting the density profile outwards [52]. The pedestal density height slightly increases while the height of the temperature significantly decreases, resulting on a lower pressure pedestal height (Fig. 3 in [53]).

On the other hand, impurity seeding can increase the relative pedestal pressure height by radiating input power away from the scrape-of-layer region, as observed at ASDEX-Upgrade [54] and JET [55, 56]. This method has been observed to significantly increase the steepness of the electron temperature while slightly reducing the steepness of the electron density (Fig. 3 in [54], reproduced in Fig. 2.4) as desired. In addition, the electron density profile can be shifted inwards by
exciting peeling-balloning modes in the pedestal as in DIII-D [57] or by reducing recycling by injecting Lithium as in NSTX [58,59].

2.4 Summary

We provide a new way to deduce directly the pedestal radial flux for non-trace impurities from measurements currently available. One of its main advantages is that it conveniently bypasses the computationally demanding kinetic calculation of the full bulk ion response by expressing the latter in terms of the poloidal impurity flow.

The neoclassical radial impurity flux has two components. The direction of
the first is shown to be related to the impurity in-out asymmetry and the poloidal flow direction, both obtainable via change-exchange recombination spectroscopy. Inboard impurity accumulation with poloidal flow in the direction of the magnetic field or outboard impurity accumulation with opposite poloidal flow direction are desirable.

The direction of the second term depends on the relative slope of the main ion density and temperature profiles, which can be estimated by those of electrons and impurities and thus measured by Thomson scattering and charge-exchange spectroscopy respectively. A bulk ion temperature profile more than twice as steep as the density is shown to lead to impurity removal and fuel absorption by this term.

The novel measuring method can be used to optimize tokamak operation to reduce if not prevent impurity accumulation while providing natural fueling. For instance, the optimal H-mode type and parameters can be selected by identifying ‘a posteriori’ the most beneficial physical behavior from a profile database.

In addition, our methodology may inspire the implementation of experimental techniques to actively and favorably modify the profiles, as well as make further measurements of their global effect on impurity confinement. For instance, toroidal rotation and ICRF minority heating can be used to push impurities outwards or inwards respectively. Moreover, mode excitation and scrape-of-layer high density reduction via impurity seeding can lead to a stronger and weaker radial variation of the electron temperature and density, respectively.
Chapter 3

Radial impurity flux measuring method with plasma heating in general geometry


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CHAPTER 3. RADIAL FLUX WITH HEATING IN GENERAL GEOMETRY

3.1 Introduction

The transport of highly charged impurities through the pedestal and their accumulation in the core of the plasma can produce significant energy losses. This can compromise the performance of tokamaks that resemble the ITER tungsten divertor, such as ASDEX-Upgrade and JET-ITL, or have molybdenum divertors, such as Alcator C-Mod. Neoclassical theory is expected to and is generally assumed to properly treat phenomena that are lower order in a gyroradius expansion, such as flow on a flux surface. However, in the pedestal higher order cross field heat transport is expected to be reduced as well due to the strong shear of the pedestal electric field.

An impure tokamak edge was originally modeled by allowing the friction of the highly charged collisional impurity species with the banana, plateau or Pfirsch-Schlüter main ions to compete with the parallel electric field and impurity pressure gradients. This self-consistent low flow ordering model was soon expanded to allow for large toroidal flows of the order of the impurity thermal velocity. Due to the centrifugal force generated, the inertial term should also be retained in this case. Subsequently, the influence of energetic ions produced by neutral beam injection (NBI) or heating by ion cyclotron resonance heating (ICRH) was considered.

The evaluation of the radial impurity flux in all of the models mentioned appears to require a computationally demanding kinetic calculation of the full bulk ion response that enters, as analytic calculations can only be performed in simple limits. However, an alternative formulation at large aspect ratio and low flows has recently been formulated that allows measuring the pedestal radial impurity flux directly from available diagnostics.

Its main advantage is that it conveniently bypasses the kinetic calculation, by expressing the radial impurity flux in terms of the measured impurity poloidal...
flow and the in-out impurity density asymmetry along with the relative radial gradients of the main ion temperature and density. The impurity mean flow, density and temperature can be measured via change-exchange recombination spectroscopy \cite{16,30,46} for intrinsic impurities up to argon (e.g. boron and carbon). The experimental challenges posed by the multiple charge states exhibited by some highly-charged impurities \cite{8} (e.g. molybdenum and tungsten) may possibly be overcome by using bolometric, ultraviolet, soft X-rays, or perhaps even on X-ray crystal spectrometer with poloidal views, as used for different argon charge states \cite{48}. In addition, the main ion temperature and density can be estimated by the impurity temperature and electron density as measured by charge-exchange recombination spectroscopy and Thomson scattering respectively, due to ion-impurity temperature equilibration and quasineutrality \cite{2}.

This novel technique provides insight on how to optimize tokamak operation to reduce impurity accumulation, and perhaps to prevent it while providing fueling. For example, the optimal H-mode type and parameters can be selected by identifying from a profile database ‘a posteriori’ the most beneficial physical behavior, as explained in \cite{2}. Moreover, this methodology may inspire the implementation of experimental techniques to actively and favorably modify the profiles. For instance, a stronger and weaker radial variation of the electron temperature and density, respectively, may be obtained by peeling-balloning mode excitation \cite{57} or scrape-of-layer density reduction \cite{50,53} via impurity seeding \cite{54}.

In this chapter, the original measuring method that we put forth \cite{2} is systematized and generalized to allow for large flows with an arbitrary poloidal electric field for general tokamak cross sections. The main extensions of this chapter beyond the calculations of Chapter 2 are thus the following:

- First, the flow need no longer be small compared with the impurity thermal velocity.
- Second, the presumption that the parallel gradient of electrostatic potential
CHAPTER 3. RADIAL FLUX WITH HEATING IN GENERAL GEOMETRY

has to be given by a flux function multiplied by the parallel gradient of the
impurity density is relaxed, giving a more general derivation.

- Third, arbitrary aspect ratio and shape are accommodated.

These extensions are motivated in part by the fact that ICRF minority heating and
toroidal rotation can also be used to actively and favorably modify the impurity
in-out asymmetry that affects the radial impurity flux [2], by pushing impurities
inwards or outwards respectively. This has been not only theoretically [25, 27]
but also experimentally proven [60]. In addition, the arbitrary aspect ratio and
poloidal cross section formulation we develop here is crucial, as it avoids the need
to computationally solve the bulk ion kinetic problem for which there are no known
general analytical solutions.

In Sec. 3.2, the methodology to bypass the kinetic calculation is presented more
generally than in [2]. In Sec. 3.3.1, the impurity flux for large flows and general
poloidal cross section is derived. In Sec. 3.3.2, simplified expressions for small
flows and arbitrary cross section are evaluated. These expressions are expanded
in the large aspect ratio limit for insight and comparison to earlier results. Section
3.4 briefly summarizes our results.

3.2 Radial impurity flux measuring method from
available measurements

The plasma is taken to be composed of banana regime electrons and lowly-charged
main ions (subscript $i$), together with a collisional highly-charged non-trace im-

O purity ($z$) [2]. Each species has density $n$, temperature $T$, pressure $p = nT$, mass
$M$, charge $z$, mean flow $V$, and particle flux $\Gamma = nV$. Note that heavy impurities
can be non-trace despite their very low concentrations. For instance, the measured
0.03% density concentration of Molybdenum (Mo) on Alcator C-Mod [19] can lead
to impurities affecting the bulk ion dynamics,

\[ z_{\text{eff}, \text{Mo}} = z_{\text{Mo}}^2 \frac{n_{\text{Mo}}}{n_e} = 0.53 \sim 1, \]

where full ionization has been assumed for illustration purposes \((z_{\text{Mo}} = 42)\). The model is also applicable in the trace limit, especially given the observed 0.5% density concentration of Boron \([19]\) leading to a \(z_{\text{eff}, \text{B}} = 0.125\).

Temperature equilibration between impurities and main ions is assumed, with the background ion temperature exhibiting negligible poloidal variation. However, the influence of a poloidally varying distribution due to fast minority ions or impurity seeding is included by allowing an arbitrary poloidal electric field that is large enough to affect the parallel impurity dynamics as in \([27]\). For instance, fast ions produced by ICRH tend to concentrate on the outboard side, due to the mirror force effect on their increased perpendicular velocity. Quasi-neutrality then forces the highly charged impurities towards the inboard side \([61]\).

### 3.2.1 Radial impurity flux

Under these assumptions, the friction force exerted on the impurities by the bulk ions in the direction parallel (||) to the magnetic field \(B\) is \([27]\)

\[ F_{z||} = \frac{n_z}{B} M_i \langle n_i \rangle \left[ \frac{v_{iz}}{n_z} \right] \left[ -\frac{cT_i}{z_i e} \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) + B^2 \left( \frac{u}{\langle n_i \rangle} - \frac{K_z}{n_z} \right) \right] \]  

\[(3.1)\]

for arbitrary aspect ratio and poloidal cross section; where \(e\) and \(c\) are the magnitude of the electron charge and the speed of light respectively. The poloidal magnetic flux is \(2\pi \psi\). The reader is referred for details to Chapter \([5.3]\), where \((3.1)\) can be recovered by substituting \((5.29)\) into \((5.35)\) and neglecting the impurity diamagnetic and radial flow effects, containing the radial derivative of impurity parameters.

The flux surface average of any quantity \(S\) is given by

\[ \langle S \rangle = \frac{\oint S \frac{d\theta}{B \nabla \psi} \cdot \oint \frac{d\theta}{B \nabla \psi} \right. \]

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where $\theta$ is the poloidal angle coordinate. Since the bulk ion temperature is taken to be a flux function, the collision frequency of bulk ions with impurities is divided by the impurity density, $n_z/n_s$, is a flux function as well (Eq. (2) in \[2\]). Furthermore, the product of the toroidal magnetic field $B_t$ and the major radius $R$, $I = RB_t$, and the constant of integration from the conservation of impurity particles,

$$K_z = n_z \mathbf{V}_z \cdot \nabla \theta/B \cdot \nabla \theta,$$

are also flux functions. The flux function $K_z$ is the only remnant in (3.1) of the impurity flow \[27\],

$$\mathbf{V}_z = -c \frac{\partial \Phi}{\partial \psi} R^2 \nabla \zeta + K_z n_z B,$$

(3.2)

since the $\mathbf{E} \times \mathbf{B}$ cancelled with that of the bulk ions. Here $\Phi$ is the electrostatic potential and $\zeta$ the toroidal angle variable.

One of the main aims of this chapter is to avoid the need to numerically solve for the background ion kinetic response $h_i$ (see Section 2.2.2) appearing in (3.1) via the following integral over main ion velocity space $\mathbf{v}$,

$$u = \frac{3\sqrt{\pi}}{\sqrt{2}} \frac{T_i^{3/2}}{M_i^{3/2}} \int \frac{d^3 \mathbf{v}}{B v^3} h_i.$$ 

This integral is also a flux function for banana main ions \[15\].

### 3.2.2 Novel methodology for direct measurement

The parallel friction (3.1) can be expressed as a function of dimensionless variables as follows:

$$F_{zi||} = \frac{n_z}{B} \langle T_z \rangle \langle \mathbf{B} \cdot \nabla \theta \rangle \left( g + b^2 U - \frac{k}{\eta} \right).$$

(3.3)

The poloidal variation of the dimensionless impurity density, $n = n_z/(n_s)$, and the square of the magnetic field, $b^2 = B^2/(B_t^2)$, are retained; while the contributions of the fluid

$$g = -\eta I \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right),$$

(3.4)
CHAPTER 3. RADIAL FLUX WITH HEATING IN GENERAL GEOMETRY

and kinetic bulk ion responses

\[ U = \eta \frac{z_i e \langle B^2 \rangle}{cT_i \langle n_i \rangle} u \]  

(3.5)

are flux functions. Here, the positive flux function \( \eta \) in (3.4) and (3.5) indicates the importance of collisions,

\[ \eta = \frac{1}{\epsilon R} \frac{cM_i}{z_i e} \left( B \cdot \nabla \theta \right) n_z \langle T_z \rangle \sim \rho_{pi} \lambda_z, \]

where \( \rho_{pi} \) is the main ion poloidal Larmor radius and \( \lambda_z \) is the impurity mean free path taking into account both like and unlike collisions.

Conventionally [15, 23–27], the dimensionless flux function related to \( K_z \) and hence to the impurity poloidal flows,

\[ k = \eta \frac{z_i e \langle B^2 \rangle}{cT_i \langle n_i \rangle} n_z V_z \cdot \nabla \theta, \]  

(3.6)

is expressed as a function of \( g \) and \( U \) by flux surface averaging the parallel momentum equation. However, it is wiser to note [2] that while the calculation of \( U \) generally requires a computationally demanding calculation, \( g \) and \( k \) can be obtained from diagnostics currently available. Indeed, the sign of \( g \) depends on the relative slope of the main ion density and temperature profiles, which can be estimated by those of electrons and impurities as measured by Thomson scattering and charge-exchange spectroscopy, respectively. In addition, the sign of \( k \) depends on the poloidal impurity flow direction, obtainable via charge-exchange recombination spectroscopy [29]. Consequently, it is convenient to bypass the kinetic calculation by using the solubility condition for (3.3) to express \( U \) as a function of \( g \) and \( k \) instead, as we do in the following section.

3.3 Formulae for general geometry

The focus of this section is to derive the algebraic expressions for general geometry required for a more accurate measurement of the pedestal radial impurity
flux. The expansion of the model to allow for large flows, plasma heating, and impurity seeding is required to make detailed experimental studies of the effect of techniques that actively attempt to prevent impurity accumulation. This is followed by simplified expressions valid for low flows and adiabatic electrons and bulk ion responses in general geometry. These expressions reduce to those in \cite{2} at large aspect ratio.

\subsection{3.3.1 Large flows}

The solubility constraint that allows to obtain a simple relation among (3.4), (3.5) and (3.6) when inertial effects are included is

$$\langle BF_{z||} \rangle = 0; \quad (3.7)$$

which follows \cite{27} by flux surface averaging the parallel momentum equation,

$$m_z n_z V_z \cdot \nabla V_z \cdot B + z_z n_z e \nabla || \Phi + T_z \nabla || n_z = F_{z||}, \quad (3.8)$$

multiplied by $\frac{B}{n_z}$. This multiplication factor has been chosen in order to make the flux surface averaged inertial contribution vanish when the impurity diamagnetic flow and the radial impurity flow are neglected, as explained in detail in Appendix \text{[B.1]} In addition, the solubility constraint in (3.7) allows for the electrostatic potential to be affected by plasma heating effects and impurity seeding, because $\langle B \cdot \nabla Q \rangle = 0$ for any single valued function $Q (\psi, \theta)$.

Substituting the parallel friction (3.3) into the solubility constraint (3.7), a relationship among $g$, $U$ and $f$ is obtained. In contrast to previous references, it is solved for the kinetic bulk ion response, which cannot be directly measured by Thomson scattering or charge-exchange recombination spectroscopy:

$$U = \frac{b^2}{n} k - g. \quad (3.9)$$

The new expression for the parallel friction, with $U$ eliminated, is

$$\frac{BF_{z||}}{n_z \langle T_z \rangle \langle B \cdot \nabla \theta \rangle} = g (1 - b^2) + k \left( \frac{b^2}{n} \frac{\langle b^2 \rangle}{n} - \frac{b^2}{n} \right). \quad (3.10)$$
CHAPTER 3. RADIAL FLUX WITH HEATING IN GENERAL GEOMETRY

It allows us to calculate the radial impurity flux,

$$\frac{\langle \mathbf{z}_\perp \cdot \nabla \psi \rangle}{z \varepsilon (B^2)} = - \langle B^2 \rangle \left\langle \frac{F_{z\parallel}}{B} \right\rangle = \left\langle \frac{BF_{z\parallel}}{n} (1 - \frac{n}{b^2}) \right\rangle,$$

where the solubility constraint (3.7) has been applied.

After some algebra, the radial impurity flux can be expressed as a function of measurements currently available as follows:

$$\frac{\langle \mathbf{z}_\perp \cdot \nabla \psi \rangle}{z \varepsilon (B^2)} = g \left( 1 - \left\langle \frac{n}{b^2} \right\rangle \right) + k \left( 1 - \left\langle \frac{b^2}{n} \right\rangle \right); \quad (3.11)$$

where

$$1 - \left\langle \frac{n}{b^2} \right\rangle = \left\langle \left( 1 - \frac{1}{b^2} \right) (n - b^2) \right\rangle = \left\langle \frac{(b^2 - 1) (n - 1)}{b^2} \right\rangle - \left\langle \frac{(b^2 - 1)^2}{b^2} \right\rangle \quad (3.12)$$

and

$$1 - \left\langle \frac{b^2}{n} \right\rangle = \left\langle \left( 1 - \frac{1}{n} \right) (b^2 - n) \right\rangle = \left\langle \frac{(n - 1) (b^2 - 1)}{n} \right\rangle - \left\langle \frac{(n - 1)^2}{n} \right\rangle. \quad (3.13)$$

Note that for low field side impurity accumulation, which can be diagnosed by charge exchange recombination spectroscopy, both (3.12) and (3.13) are negative. In this case, just by measuring the signs of $g$ and $k$, one can determine if the corresponding flux contributions are inward or outward.

### 3.3.2 Low flows

The previous solubility constraint (3.7) and results (3.11) also apply to the case of low flows,

$$z z_n e \nabla || \Phi + T_i \nabla || n_z = F_{z\parallel}, \quad (3.14)$$

where the inertial term can be ignored. In the case that the electrostatic potential is only determined by an impurity species and Maxwell-Boltzmann electrons and main ions, there is another solubility constraint that allows us to simplify the expression for the radial impurity flow further, namely

$$\left\langle BF_{z\parallel} \right\rangle = 0, \quad (3.15)$$
which is obtained by flux surface averaging the parallel momentum equation (3.14) multiplied by $B$. In particular, a relationship between the poloidal derivative of the electrostatic potential and the electron and main ion densities can be obtained from their Maxwell-Boltzmann response, i.e. $n = \langle n \rangle \exp \left[ -\frac{ ze(\Phi - \langle \Phi \rangle)}{T} \right]$, since their temperatures are taken to be flux functions. The poloidal variation of the potential can then be related to that of the impurity density by subtracting from the quasineutrality equation its flux surface average and taking the poloidal derivative to find

$$\frac{z_e}{T_i} \nabla_{||} \Phi = \frac{z_e \nabla || n_z}{z_i n_i + \frac{T_i}{z_i} n_e},$$  

(3.16)

from which the solubility condition in (3.15) can be derived.

Using the solubility constraint in (3.15), the kinetics effects are expressed in terms of directly measurable quantities as

$$U = \frac{k - g}{\langle nb^2 \rangle}.$$

Substituting this back into (3.3), an expression for the parallel friction as a function of measurements currently available is obtained to be

$$\frac{BF_{zi\parallel}}{\langle T_z \rangle \langle B \cdot \nabla \theta \rangle} = n_z \left[ g \left( 1 - \frac{\nu^2}{\langle nb^2 \rangle} \right) + k \left( \frac{\nu^2}{\langle nb^2 \rangle} - \frac{\nu^2}{n} \right) \right].$$  

(3.17)

The new solubility constraint can be used to simplify the calculation of the radial impurity flux to

$$\frac{\langle \Gamma_z \cdot \nabla \psi \rangle}{cz_e \langle B^2 \rangle} = -\langle B^2 \rangle \left( \frac{F_{zi\parallel}}{B} \right) = \langle BF_{zi\parallel} (1 - \frac{1}{b^2}) \rangle.$$

After some algebra, a new expression of the radial impurity flux as a function of measurements currently available is found to be

$$\frac{\langle \Gamma_z \cdot \nabla \psi \rangle}{cz_e \langle n_z \rangle \langle T_z \rangle \langle B \cdot \nabla \theta \rangle} = \frac{n_z}{\langle nb^2 \rangle} - \frac{n_\psi}{b^2} + k \left( 1 - \frac{1}{\langle nb^2 \rangle} \right).$$  

(3.18)

By multiplying the parallel momentum equation by $\frac{B}{nz}$ and flux surface averaging, using expression (3.17) for the friction, a relationship among $g$ and $k$ follows...
that allows us to recover exactly the large flow radial impurity flux (3.11):

$$g \left( 1 - \frac{1}{\langle nb^2 \rangle} \right) + k \left( \frac{1}{\langle nb^2 \rangle} - \frac{\langle b^2 \rangle}{n} \right) = 0.$$  

This also implies that the expression for the parallel friction in the parallel momentum equation for large flows (3.10) is the same as for low flows (3.17) if inertia is negligible and (3.16) is valid.

The radial impurity flux for low flows (3.18) can be rewritten by using (3.12) to find

$$\langle \Gamma_z \cdot \nabla \psi \rangle = k \frac{\langle (b^2 - 1)(n - 1) \rangle}{\langle nb^2 \rangle} - g \left( \frac{\langle 1 - b^2 \rangle^2}{b^2} \right) - g \left( n - 1 \right) \frac{\langle b^2 - 1 \rangle}{\langle nb^2 \rangle} \frac{\langle (n - 1)(b^2 - 1) \rangle}{\langle b^2 \rangle}.$$  

The large aspect ratio limit appearing in [2] can be recovered by dropping higher order terms to find

$$\langle \Gamma_z \cdot \nabla \psi \rangle = k \frac{\langle (b^2 - 1)(n - 1) \rangle}{\langle nb^2 \rangle} - g \left( \frac{\langle 1 - b^2 \rangle^2}{b^2} \right).$$  

The first term of the radial impurity flow is then outward when there is inboard impurity accumulation with poloidal flow in the direction of the magnetic field, or outboard impurity accumulation with opposite poloidal flow direction. The second term is outwards for a bulk ion temperature profile more than twice as steep as the density. In this case natural fueling occurs [2].

### 3.4 Summary

We provide a systematic method of evaluating the pedestal radial flux for non-trace impurities in arbitrary geometry from measurements currently available. One of its main advantages is that it conveniently bypasses the computationally demanding kinetic calculation of the full bulk ion response. Indeed, the method
consists of using the solubility constraint to remove this kinetic response instead of the poloidal impurity flow, as the latter can be directly measured by charge-exchange recombination spectroscopy.

The large aspect ratio limit was considered originally [2] to simply illustrate how to directly calculate the radial impurity flow from available diagnostics. Attention was drawn to the diagnostics required to measure each of the physical parameters involved, such as Thomson scattering and charge-exchange recombination spectroscopy, with a view to motivating the expansion of present databases [20, 29–31]. The focus of the present article is to provide the means for a more accurate measurement of the pedestal radial impurity flux, by extending it to a realistic tokamak situation with arbitrary aspect ratio and general geometry.

The reader is referred to [2] for a more detailed identification of the optimal physical phenomena leading to an outward radial impurity flux, and consequently optimum plasma fueling. Experimental techniques that could actively trigger these beneficial phenomena were also suggested, including impurity seeding, neutral beam injection and ion cyclotron resonance heating of minority ions, even though they were not included in the low flow model [2]. In contrast, the model presented in this chapter permits for seeding and toroidal flows of the order of the impurity thermal velocity. It thus remains valid when plasma heating techniques are used to actively and favorably modify the radial impurity flux. Consequently, our results could substantially improve fusion performance by optimizing tokamak operation by reducing and perhaps preventing impurity accumulation, and thereby provide better fueling.
Chapter 4

Theoretical explanation of I-mode impurity removal and energy confinement


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4.4 Insight into I-mode explanation ............................ 74
4.1 Introduction

A key experimental discovery towards making clean, safe and unlimited fusion energy economically competitive took place 35 years ago \[17\]. It was observed that the power produced by a given reactor could suddenly be almost quadrupled at a constant input power. This high confinement mode (H-mode) operation was characterized by both higher energy and impurity particle confinement than exhibited by the low confinement mode (L-mode) regime.

A summary of the progress made towards a theoretical understanding of the physics behind the L-H transition, that could lead to even further improvements of fusion power plant performance, can be found in several review papers \[21,62–64\]. Briefly, the radial electric field was predicted \[65\] to have an important role in this transition. In the L-phase, the radial electric field is flat and weakly negative. Its radial profile is measured to become significantly negative at the transition, before the electron temperature and density appreciably change \[66\]. Finally, while a transport barrier in temperature and density suddenly forms, the radial electric field may continue to evolve \[66–68\]. As a result, the radial electric field becomes more negative in H-mode; especially in the pedestal, the region near but still inside the separatrix. The development of the radial electric field has even been observed in stellarators \[69–71\] as well as in tokamaks.

During the L-H transition, the level of turbulence was measured to drop sharply \[72\] at the pedestal and the turbulent particle flux observed to collapse (Figure 7 of \[73\]). Turbulence stabilization by sheared flows was expected \[74\], proposed \[18\] and experimentally confirmed \[75\]. The sheared $E \times B$ flow leads to the breakup of turbulent eddies in the pedestal. Indeed, the lower amplitude of the turbulence may be only large enough to affect heat transport and other higher order phenomena in a poloidal Larmor radius expansion. Neoclassical collisional theory is normally assumed \[2,3,15,23,27\] to properly explain lower order phenomena,
such as flows.

The high energy confinement of the H-mode is extremely beneficial to the commercialisation of fusion energy. Nevertheless, the high impurity confinement can lead to large radiative energy losses \[9\] that compromise the performance of high charge number metal wall tokamaks, such as Alcator C-Mod \[14\], ASDEX-Upgrade \[13\] and JET ITER-Like Wall \[10\]–\[12\].

Less than a decade ago, an improved confinement mode (I-mode) was experimentally observed at Alcator C-Mod \[19\], with high energy confinement but somewhat lower impurity confinement. I-mode is not only a breakthrough solution to the core high charge number impurity accumulation challenge, but it also may successfully prevent plasma dilution by eliminating ash from the core. A radial electric field well of similar depth and slightly larger width than for H-mode has been measured \[29\] for I-mode, where the shear of both the radial electric field and the poloidal flow is stronger close to the separatrix.

The presence of a weakly coherent mode in I-mode was originally proposed \[19\] as a method to distinguish it from the H-mode. Nonetheless, modes exhibiting the same characteristics as an I-mode with high energy confinement and low particle confinement but without the detection of the weakly coherent mode have been observed, perhaps due to its extreme spatial localization. As a consequence, a reliable criterion to distinguish I-mode from H-mode would be beneficial. Most importantly, a better understanding and control of the physical phenomena responsible for impurity removal in I-mode may lead tokamak design to further improvements in fusion performance.

Recently, the first method to measure the neoclassical radial impurity flux directly from available diagnostics, such as charge exchange recombination spectroscopy and Thomson scattering, was proposed \[2\]–\[3\]. One of its main advantages is that it bypasses the computationally demanding kinetic calculation of the full bulk ion response. The method was originally formulated at large aspect ratio and
low flows \[2\]. It was then systematized and generalized to allow for large flows with an arbitrary poloidal electric field for general geometry \[3\]. This procedure also allows the inclusion of ICRF minority heating and toroidal rotation effects that can be used to actively and favorably modify the radial impurity flux to prevent impurity accumulation, as explained in \[2\].

In this chapter, the direction of the neoclassical radial impurity flux in I-mode is evaluated with experimental data \[19, 20, 29\]. An inward neoclassical radial impurity flux would make the weakly coherent mode solely responsible for pushing impurities out. However, we find that the neoclassical theory correctly predicts an outward radial impurity flux, without the need of invoking anomalous mechanisms. Furthermore, we propose a new additional feature to distinguish H-mode and I-mode based on the direction of the neoclassical radial impurity flux, being inwards for the former and outwards for the latter. The presence of strong $E \times B$ shear may explain the high energy accumulation observed in both modes, due to the decorrelation of the turbulence and its reduction.

### 4.2 Neoclassical radial impurity flux

The plasma is taken to be composed of Maxwell-Boltzmann banana regime electrons (subscript $e$) and main ions ($i$), together with a collisional highly-charged non-trace impurity ($z$) \[2\]. Each species has density $n$, temperature $T$, pressure $p = nT$, mass $M$, charge $z$, mean flow $V$ and particle flux, $\Gamma = nV$. Toroidal flows are allowed to be on the order of the thermal impurity flow. Finally, the influence of a poloidally varying effects due to ICRH fast minority ions or impurity seeding is included, as in \[27\], by allowing an arbitrary poloidal electric field that is large enough to affect the parallel impurity dynamics.

The neoclassical pedestal radial impurity flux in general geometry can be ex-
pressed as a function of available measurements as \[3\]
\[
\frac{\langle \Gamma_z \cdot \nabla \psi \rangle}{c (B \cdot \nabla \theta) (T_i) (n_i)} = g A + k A;
\]
where \( I = RB_t \), with \( R \) the major radius and \( B_t \) the toroidal component of the magnetic field \( B \). The poloidal angle and magnetic flux are denoted by \( \theta \) and \( 2\pi \psi \), the speed of light by \( c \) and the magnitude of the electron charge by \( e \). The flux surface average of a quantity \( Q \) is defined as
\[
\langle Q \rangle = \frac{\oint Q d\theta}{\oint d\theta} = \frac{\oint Q d\vartheta}{2\pi};
\]
where \( \vartheta \) is a modified poloidal angle coordinate, satisfying \( d\vartheta \langle B \cdot \nabla \theta \rangle = d\theta \langle B \cdot \nabla \theta \rangle \).

In the following dimensionless flux functions appearing from the right hand side of (4.1),
\[
g = -\xi I \left( \frac{d \ln \langle n_i \rangle}{d\psi} - \frac{1}{2} \frac{d \ln T_i}{d\psi} \right);
\]
and
\[
k = \xi z_i e \langle B \rangle \frac{n_z}{c T_i} \frac{V_z \cdot \nabla \theta}{B \cdot \nabla \theta},
\]
the positive flux function \( \xi \) indicates the importance of collisions, \( 0 \leq \frac{\xi}{R} = \frac{1}{c M_i} \langle n_i \rangle \frac{\nu_{iz}}{n_z} \frac{T_i}{T_z} \sim \frac{\rho_{pi}}{\lambda_z} \). Here \( \epsilon \) is the inverse aspect ratio (minor over major radius), \( \nu_{iz} \) the collisional frequency of background ions with impurities \( 2 \), \( \rho_{pi} \) the main ion poloidal Larmor radius, and \( \lambda_z \) the impurity mean free path taking into account both like and unlike collisions.

The two asymmetry factors in (4.1),
\[
A = 1 - \langle \frac{n}{b^2} \rangle = \left( \frac{n - 1}{b^2} \right) - \left( \frac{b^2 - 1}{b^2} \right);
\]
and
\[
A = 1 - \langle \frac{b^2}{n} \rangle = \left( \frac{n - 1}{n} \right) - \left( \frac{n - 1}{n} \right),
\]
depend on the poloidal variation of the dimensionless impurity density, \( n = \frac{n_z}{(n_z)} \), with respect to that of the square of the normalized magnetic field, \( b^2 = \frac{B^2}{(B^2)} \).
In this section, the sign of each of the radial impurity flux components is determined from illustrative I-mode experimental measurements. A summary of the signs of each of the terms in (4.1) is provided in Table 4.1 together with the measurements leading to these conclusions.

First, the sign of \( g \) in (4.2) depends on the relative slope of the main ion density and temperature profiles, which can be estimated \cite{2} by using those of the electrons and impurities, respectively, as measured by Thomson scattering and charge-exchange spectroscopy. The availability of an extensive Thomson scattering database \cite{19} for the electron density and temperature profiles, normally assumed to be of the same order as the bulk ion temperature \cite{2,3,15,23,27}, is used here to estimate \( g \). Perhaps in the future the radial impurity flux measuring technique proposed in \cite{2,3} will encourage an extension of the impurity temperature database.
In particular, L–I transitions become very distinct on C-Mod mode exist and can be clearly identified in most cases. C-Mod has shown that distinct transitions from L-mode to I-regime solely by its confinement quality factor (a noticeable increase in density, making identification of the region due to core radiation from high temperatures). In global particle confinement (∼ decreases gradually throughout the shot with its average value set by a feedback loop for density control with cryopumping) in the core density. The external fuelling rate (figure 4.1) also features a transition to ELM-free H-mode at the H-mode transition the density and ion temperature (time slices are indicated by vertical lines). The transition to a transient ELM-free H-mode (at ∼ 27 GHz cutoffs, i.e. the 110 GHz reflectometer channel (not available from CXRS, they have also been found to increase significantly with the increase in pedestal temperature). Noticeable, but often weak, breaks in Nucl. Fusion (2010) 105005 D.G. Whyte et al.

by using charge exchange recombination spectroscopy to better advantage.

A bulk ion temperature profile more than twice as steep as the density profile is needed for g to be negative, η ≡ d ln T_i / d ln n_e ~ d ln T_e / d ln n_e > 2. As illustrated in Fig. 3 in [19] (Fig. 4.1), the I-mode generally displays a similar electron temperature gradient and a weaker electron density gradient than the H-mode. Furthermore, the I-mode is characterised by a stronger temperature gradient than L-mode for a similar density gradient, as also shown on Fig. 1 in [47] (Fig. 4.2). This translates into I-mode generally having a significantly smaller g than H-mode and L-mode.

After analyzing the Alcator C-Mod Thomson scattering data (Fig. 13 of [19]), with B × ∇B away from the X-point; it was observed that more than 97% of the
roughly one hundred I-modes under study exhibited a negative $g$. We will highlight shot number 1120921026, for which charge spectroscopy data is available \cite{20, 29}. For this shot, $g$ is negative as it is in the majority of I-mode discharges.

Second, the sign of $k$ \cite{4, 3} is shown to be related to the poloidal ($p$) impurity flow direction, obtainable via change-exchange recombination spectroscopy. The database for charge-exchange spectroscopy I-mode data is sparse. Here we use the shot 1120921026 for illustrative purposes because a complete data set has been published \cite{20, 29}. Close to the separatrix, the poloidal flow is in the direction...
poloidal and toroidal viewing optics. The bottom panel shows the radial electric field obtained using equation (a) GP-CXRS measurements \((E_{\rho})\) of the radial electric field and their components at the midplane in I-mode (adapted from Fig. 4 of [29]).

opposite to the magnetic field and hence \(k < 0\) (Fig. 4 of [29] and Fig. 4.8 in [49], adapted in Fig. 4.3 and Fig. 4.4 respectively). Due to the poloidal field reversal in I-mode, this behaviour is expected to be typical.

Third, note that the second terms of the latter expression of \(A\) in (4.4) and \(\mathcal{A}\) in (4.5) are always negative. However, the sign of the first terms depends on the poloidal variation of the impurity density, which can be measured via charge-exchange recombination spectroscopy \([16,30,46]\), with respect to that of the known magnetic field squared. The low and high field side midplane diagnostics on Alcator C-Mod detect a larger boron density on the outboard than on the inboard side for I-mode shot 1120921026 (Fig. 18 of [20], adapted in Fig. 4.5). Based on these measurements, the quantity that is flux surface averaged in both first terms of \(A\) and \(\mathcal{A}\), \((n - 1)(b^2 - 1)\), is also negative.

When considering for illustrative purposes a first-order cosinusoidal profile for the dimensionless magnetic field, \(b^2 = 1 - 2\epsilon \cos \vartheta\), and a first-order Fourier profile for the dimensionless impurity density, \(n = 1 + n_c \cos \vartheta + n_s \sin \vartheta\); the asymmetry

---

**Figure 4.3:** Charge-exchange recombination spectroscopy measurements \((B^{5+})\) of the radial electric field and their components at the midplane in I-mode (adapted from Fig. 4 of [29]).
Figure 4.4: Inboard and outboard impurity density and poloidal flow radial profiles in a reversed field I-mode (adapted from Fig. 4.8 in [49]).

factors [27] are negative for outboard \((n_c > 0)\) impurity accumulation,

\[
A = 1 - \left( \frac{n}{b^2} \right) = -\epsilon (n_c + 2\epsilon) < 0
\] (4.6)

and

\[
A = 1 - \left( \frac{b^2}{n} \right) = -n_c\epsilon - \frac{n_c^2 + n_s^2}{2} < 0
\] (4.7)

to second-order accuracy.

In conclusion, both terms of the neoclassical radial impurity flux in (4.1) are positive and thus outwards in I-mode, as indicated by the signs of each of its components as summarized in the last column of Table 4.1.

Under neoclassical assumptions, while the impurities go outward in I-mode, the main ions that fuel the plasma must go inward to preserve ambipolarity,

\[ z_i \langle \mathbf{\Gamma}_i \cdot \nabla \psi \rangle = -z_z \langle \mathbf{\Gamma}_z \cdot \nabla \psi \rangle. \]

Note that the contribution of the radial electron flux has been neglected since

\[
\frac{\Gamma_e \cdot \nabla \psi}{z_e \Gamma_e \cdot \nabla \psi} \sim \frac{\rho_e}{\rho_e} \sim \frac{\Omega_c \nu_e}{\rho_e \nu_z} \sim \sqrt{\frac{m_e}{m_i}} \ll 1
\]

\[ ^1\text{For details, the reader is referred to (5.60) and (2.1).} \]
CHAPTER 4. EXPLANATION OF I-MODE IMPURITY REMOVAL

Figure 4.5: Inboard and outboard impurity density profiles for an illustrative I-mode (adapted from Fig. 18 of [20]).

One might explain the absence of density build up in I-mode by supposing the charge outflow of impurities ($\propto z_i n_i$) balances the charge influx of bulk ions ($\propto z_e n_e$), even though $z_i^2 n_i \sim z_e^2 n_e$ is traditionally assumed [15, 23, 27] to make the algebra tractable.

The rotational effects included in the model in [3] make it possible for both terms ($gA$ and $kA$) to be simultaneously outwards for low field side impurity accumulation even in the large aspect ratio limit, in contrast to [2]. For instance, when considering the illustrative profiles used to derive (4.6) and (4.7) with adiabatic background responses (Eq. (15) in [3]) and an impurity toroidal rotation with Mach number $M^2 = M_0^2 (1 + 2\epsilon \cos \vartheta) \sim 1$, the linearized parallel momentum equation can be solved (Sec. IVA of [25]) to obtain

$$n_e = 2\epsilon M_0^2 (1 + \alpha) - gk \left(1 + \alpha \right)^2 + k^2. \quad (4.8)$$

Here the large aspect ratio limit of Eq.(9) in [3] has been used and the effective
charge of impurities is given by

\[ \alpha = \frac{z_i^2 n_i}{z_i z_n} \frac{\langle n_z \rangle}{1 + \frac{n_e}{z_i n_i} T_i T_e} \lesssim 1. \]

From (4.8), it can be observed that both \( g \) and \( k \) can have the same sign for low field side impurity accumulation (\( n_c > 0 \)) as observed in I-mode due to the presence of toroidal rotation satisfying \( M_0^2 (1 + \alpha) > gk \). Recall that the magnitude of \( g \) in (4.2) becomes smaller as the impurity temperature profile gets closer to be twice as steep as the electron density, making it easier for the Mach number to compete with \( g \) in (4.8). As both \( A \) and \( A \) are expected to be negative for outboard impurity accumulation, both terms of the radial impurity flow in (4.1) can thus be simultaneously outwards as desired for I-mode operation.

### 4.4 Insight into I-mode explanation

In this section, the explanation of impurity removal in I-mode [19] and the identification criterion are discussed. Fresh insight into particle and energy confinement in I-mode is deduced here, based on recent experimental data and the radial impurity flux measuring method presented in previous sections. These observations along with our deeper theoretical understanding lead to the proposal of a new robust criterion to distinguish I-mode from H-mode.

Fig. 4.6 provides schematics of potential physical explanations of I-mode characteristics (Fig. 4.6a) and how to diagnose its presence (Fig. 4.6b). First, the axis in Fig. 4.6a represents the two ideal properties in a confinement mode: energy confinement and impurity removal, which leads also to free fueling by ambipolarity. While H and L-mode present the former and latter respectively, I-mode is the most favorable by exhibiting both as indicated by its location on the upper right corner.
(a) Physical insight into particle and energy confinement.

(b) I and H-mode classification criterion.

Figure 4.6: Pioneering \([19]\) (red) and proposed (blue) theoretical explanations of impurity and energy confinement in I-mode and identification criterion.

I-mode operation was originally believed to be associated with turbulence, as indicated in red in Fig. 4.6(a). Indeed, it was suggested that the I-mode could be identified via multi-frequency reflectometry detection of a weakly coherent mode in the pedestal \([19]\), as sketched in Fig. 4.6(b) also in red. Based on this explanation, the neoclassical radial impurity flux can be inwards in I-mode, with turbulence being solely responsible for transporting impurity outwards. However, we have shown here that outward neoclassical impurity flux occurs for I-mode, without the need of invoking any anomalous transport mechanism. Our explanation allows I-mode operation with impurity removal and good energy confinement to occur when the weakly coherent mode is not detected in agreement with observations.

The fact the neoclassical theory can correctly predict the direction of the flows in I-mode is in one way similar to the H-mode scenario. Turbulent eddies can be broken up and reduced in size by \(\mathbf{E} \times \mathbf{B}\) shear. The large negative radial electric field observed in all I-modes pedestals investigated by charge exchange
spectroscopy, becomes more strongly sheared close to the separatrix (see Fig. 4 in [29]). Consequently, the good energy confinement observed in both H and I-mode may be due to the sheared $E \times B$ flow decorrelation of the turbulence, as summarized in blue in Fig. 4.6(a).

To distinguish between I-mode and H-mode operation we propose a new criterion based on the radial impurity flux direction. We sharpen the distinction between these two operating regimes by taking advantage of the radial impurity flux measuring method first proposed for H-mode in [2,3] and here extended to include I-mode. Our new criterion is based on the radial flux direction, and consistent with experimental observations of the key physical characteristics of these confinement modes. Specifically, we find that I-mode and H-mode can be identified by having an outward and inward neoclassical radial impurity flux respectively, as illustrated in Fig. 4.6(b).

Our explanation suggests that carefully controlling the profiles in the pedestal will allow fusion relevant tokamaks to take full advantage of the desirable features of I-mode operation such as reduced heat transport, and impurity removal resulting in efficient natural fueling.
Part II

Theoretical explanation of pedestal poloidal variation, addressing the concern regarding H-mode pedestal turbulence reduction (2D: Chap. 5-7)
Chapter 5

Predictive non-linear neoclassical model for poloidal asymmetries in tokamak edge pedestals

## CHAPTER 5. EXPLANATION OF PEDESTAL POLOIDAL ASYMMETRIES

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CHAPTER 5. EXPLANATION OF PEDESTAL POLOIDAL ASYMMETRIES

5.1 Introduction and motivation

In H-mode pedestals turbulence is greatly reduced, and so is turbulent transport. In some cases neoclassical bulk transport appears to dominate, but even if turbulent bulk transport is important, impurity influx may be determined by neoclassical transport. This chapter develops an extended neoclassical impurity transport theory that is applicable to steep impurity gradients.

During the last two decades, the state-of-the-art neoclassical pedestal theories for impurity behavior \cite{15,23,25,35} have been analyzing the impurity parallel dynamics independently. In other words, the physical phenomena included were selected \cite{15} such that the interesting effects of the impurity radial flow could be self-consistently neglected for simplicity when evaluating its parallel flow and treating conservation equations. First, the collisional impurity is allowed to be non-trace, i.e. its density is taken to be large enough to affect the bulk ion dynamics by allowing the collisional frequency of bulk ions with impurities to compete with the self-collision frequency of the background. Second, the impurity and main ion flows are assumed significantly weaker than the thermal velocity of the impurities, since the characteristic perpendicular length scales are taken much larger than the impurity poloidal gyroradius. The key simplifying assumption towards neglecting the impurity radial flows relies on taking the pedestal characteristic length to be of the same order for both impurity and main ion densities. In this way the diamagnetic flow can be neglected for high charge state impurities, while it is retained for the bulk ions.

Even though retaining radial flow effects may be essential towards calculating impurity accumulation, the existing theories continue to provide valuable insight into the poloidal rearrangement within a flux function of impurities in thermal equilibrium with weakly poloidally varying background ions. The primary reason being that Helander \cite{15} proved that impurities can accumulate on the inboard side.
of a flux surface due to the friction with the background ions. His model allows the friction to compete with the potential and pressure gradient terms in the impurity parallel momentum conservation equation. The drive for this impurity density in-out asymmetry is given by the poloidal variation of the magnetic field. The inverse dependence of the bulk diamagnetic flow on the magnetic field magnitude can cause the impurity density to be higher on the high field side than on the low field side. If the impurity toroidal rotation was large enough, the inertial term should be retained and the centrifugal force could overtake the previous phenomena, causing the highly-charged impurities to concentrate on the low field side [25].

The original model with banana regime main ions [15] was extended to the Pfirsch-Schlüter [23] and plateau [24] collisionality regimes, in the hope of explaining larger impurity concentration on the high field side. However, high confinement mode edge pedestals on Alcator C-Mod [20,28,29] exhibit somewhat stronger poloidal variation than predicted by the most comprehensive neoclassical theoretical models developed to date [15,23,24,35], indicating that there may be some physical process missing from these models. This phenomenon may be amplifying the magnetic field in-out asymmetry, which is the only drive in previous theories, or acting as an additional drive. Impurity peaking at the inboard side is also observed in other tokamaks, such as ASDEX-U [30,31] and JET [32]. In addition, up-down asymmetries have also been detected on tokamaks, such as Alcator A [36], PLT [37], PDX [38], ASDEX [39], Compass-C [40] and Alcator C-Mod [41,43].

Charge-exchange recombination spectroscopy [46] is used to measure the outboard (LFS) and inboard (HFS) boron temperature, density and mean flow radial profiles in the midplane pedestal region of Alcator C-Mod. Due to uncertainties in the pedestal magnetic equilibrium reconstruction, further assumptions regarding the location of the flux surfaces are made in order to align the inboard and out-
Figure 5.1: Illustration of alignment techniques by considering different variables to be flux functions in order to match the HFS and LFS profiles in an EDA H-mode (Fig. 1 in [20]).
board radial profiles \cite{20,28,29}. Experiments \cite{20,29} indicate that the electrostatic potential and impurity temperature are not simultaneously flux functions. The total pressure alignment (Fig. 5.1(b)) leads to a weaker impurity density asymmetry than when taking the impurity temperature as a flux function (Fig. 5.1(a)) instead (see Fig. 6 of Ref. \cite{20} or Fig. 5.2), but the accumulation of boron density on the high field side is still up to six fold for pressure alignment. In this case, the boron temperature is larger on the outboard (LFS) side compared to inboard (HFS), exhibiting a weaker radial and poloidal variation than the density (see Fig. 1 and 6 of Ref. \cite{20}).

The impurity model in the following sections proposes a self-consistent two-dimensional theoretical neoclassical model for axisymmetric tokamak pedestals. In contrast to the one-dimensional previous models \cite{15,23,25,35}, the impurity parallel dynamics is affected not only by flows contained in the flux surface but also by the impurity radial flows out of the flux surface. The novel expressions for
the impurity flow and conservation equations may improve our ability to model pedestals and perhaps extend existing codes \cite{14,45} to a new dimension. More importantly, this pedestal neoclassical model with radial flows may ultimately suggest how to better control or even avoid impurity accumulation in tokamaks such as JET and ASDEX-Upgrade.

Radial flow effects become important when the impurity density exhibits very strong radial gradients. We achieve self-consistency by allowing the impurity diamagnetic drift to compete with the $E \times B$ drift, as supported by experimental observations \cite{29}. Radial and diamagnetic flow effects substantially alter the parallel impurity flow. The resulting modification in the impurity friction with the banana regime background ions impacts the impurity density poloidal variation, by acting as an amplification factor on the magnetic field poloidal variation drive. It can lead to stronger poloidal variation that is in better agreement with the observations for physical values of the diamagnetic term. In addition, the poloidally-dependent component of the radial electric field can compete with its flux surface average for the first time. Finally, compressional heating now prevents complete equilibration between impurities and the main ions, resulting in an impurity temperature in-out asymmetry. The key new physical phenomena of our model and its success in achieving stronger poloidal variation are outlined on Table 5.1 for comparison with previous models.

The remaining sections are organized as follows. Section 5.2 is devoted to experimentally justifying the new physical phenomena included in the model and the corresponding orderings for the potential and species variables. The comprehensive range of collisionality for which the orderings are self-consistent, i.e. simultaneously verified, is also presented. In Appendix C, the kinetic theory of the banana regime main ions is carefully analyzed when radial gradients of poloidally-varying variables are retained, in order to successfully calculate the parallel friction force between impurities and the background ions as a function of the impurity parallel
CHAPTER 5. EXPLANATION OF PEDESTAL POLOIDAL ASYMMETRIES

Experimental physics observed [20, 28, 29, 15, 23, 25, 35] This work

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Table 5.1: Novel physical phenomena included and poloidal asymmetries captured by the proposed neoclassical model in comparison to the state-of-the-art models developed to date.

flow. Section 5.3 contains the calculation of the impurity flow with diamagnetic and radial flow effects using conservation of impurity particles and momentum. Special attention is drawn to the new sources of poloidal variation in order to provide insight into parallel and poloidal flow measurements. It is shown in Sec. 5.4 that the generalized parallel friction modifies the impurity parallel momentum conservation equation governing the impurity density poloidal rearrangement. Finally, the results are summarized and discussed in Sec. 5.5.
5.2 Self-consistent orderings of the edge pedestal theoretical model

The theoretical pedestal model proposed here aims to explain the poloidal asymmetries in the impurity density, electrostatic potential, and impurity temperature by including the additional physical phenomena summarized on Table 5.1. This section is devoted to the development and experimental justification of the new orderings that are able to accomplish this task and provide additional physical insight within a self-consistent framework. The range of applicability of this new model overlaps and extends that of previous models [15].

5.2.1 Impure tokamak pedestal

We consider an axisymmetric tokamak pedestal composed of Maxwell-Boltzmann banana regime electrons (subscript $e$) and bulk ions ($i$) with charge number $z_i \sim 1$. The model includes a single highly charged impurity ($z$) with temperature $T_z \sim T_i \sim T_e$ and mass $M_z$ satisfying

$$\sqrt{\frac{M_z}{M_i}} \approx \sqrt{\frac{z_z}{z_i}} \gg 1.$$  \hspace{1cm} (5.1)

This impurity is assumed to be collisional (Pfirsch-Schlüter) and non-trace, so that

$$\frac{z_z^2 n_z}{z_i^2 n_i} \sim \frac{\nu_{iz}}{\nu_{ii}} \sim \frac{\nu_{zz}}{\nu_{zi}} \sqrt{\frac{z_i}{z_z}} \sim \frac{\nu_{zz}}{\nu_{ii}} \left( \frac{z_i}{z_z} \right)^{\frac{3}{2}} \sim 1.$$  \hspace{1cm} (5.2)

Here $n$ is the species density and $\nu_{12}$ the collisional frequency of species 1 with 2.

The collisional frequencies between impurities and/or main ions are given [76]
by

\[ \nu_{ii} = \frac{4\sqrt{\pi} z_i^4 e^4 n_i \ln \Lambda}{3M_i^1 T_i^2} \]

\[ \nu_{iz} = \frac{4\sqrt{2\pi} z_z^2 z_i^2 e^4 n_z \ln \Lambda}{3M_i^1 T_i^2} \]

\[ \nu_{zz} = \frac{4\sqrt{\pi} z_z^4 e^4 n_z \ln \Lambda}{3M_z^1 T_z^2} \]

and

\[ \nu_{zi} = \frac{8\sqrt{2\pi} M_i^1 z_i^2 z_z^2 e^4 n_z \ln \Lambda}{3M_z T_z^2} , \]

where \( \ln \Lambda \) is the Coulomb logarithm. Note that the collision frequencies between impurities and main ions satisfy \( 2M_i n_i \nu_{iz} = M_z n_z \nu_{zi} \).

The sizes of the collisional frequencies can be compared to find

\[ \frac{\nu_{iz}}{\nu_{ii}} = \sqrt{2} z_{\text{eff}} \sim z_{\text{eff}}, \]

\[ \frac{\nu_{zz}}{\nu_{zi}} = \frac{1}{2\sqrt{2}} \left( \frac{T_i}{T_z} \right)^{3/2} \left( \frac{M_z}{M_i} \right)^{1/2} z_{\text{eff}} \sim \left( \frac{z_z}{z_i} \right)^{1/2} z_{\text{eff}} \]

and

\[ \frac{\nu_{zz}}{\nu_{ii}} = \sqrt{2} \left( \frac{z_z}{z_i} \right)^{3/2} \left( \frac{M_i}{M_z} \right)^{1/2} z_{\text{eff}} \sim \left( \frac{z_z}{z_i} \right)^{3/2} z_{\text{eff}} \]

where \( z_{\text{eff}} = \frac{z_z n_z}{z_i n_i} \) is the effective charge of the impurities.

### 5.2.2 Strong poloidal variation

The flux surface average of a quantity \( Q \) is defined as

\[ \langle Q \rangle = \frac{\oint Q d\theta}{\oint B \cdot \nabla \theta} = \oint \frac{Q d\theta}{2\pi} ; \quad (5.3) \]

with \( B \) the magnetic field, \( \theta \) the poloidal angle variable and \( d\theta = (B \cdot \nabla \theta) d\theta \) [15].

A relationship between the poloidal derivative of the electrostatic potential, \( \Phi \), and the electron and main ion densities can be obtained from their Maxwell-Boltzmann response, i.e. \( n = \langle n \rangle \exp \left[ -\frac{ze(\Phi - \langle \Phi \rangle)}{T} \right] \), since their temperatures are taken to be lowest order flux functions. The poloidal variation of the potential can
also be related to that of the impurity density by subtracting from the quasineutrality equation its flux surface average and taking the poloidal derivative:

\[
\frac{z_i e \partial \Phi}{T_i} = \frac{z}{n_e z_i T_i e} \frac{\partial n_z}{\partial \theta} = \frac{z_i}{z} \frac{z_i^2 n_e z_i}{z_i^2 n_i} \frac{\partial \ln n_z}{\partial \theta}.
\] (5.4)

Moreover, the poloidal variation of the magnetic field, which is of the order of the inverse aspect ratio \( \epsilon \ll 1 \), is retained by considering it to be stronger than that of the potential and the electron and background ion densities. Finally, the impurity density is allowed to exhibit the strongest poloidal variation, \( \Delta \), that is taken to be of order \( \sqrt{\epsilon} \) in order to keep nonlinear effects.

The orderings for the poloidal variation of the physical quantities under consideration can thus be conveniently summarised as

\[
1 \gg \left| \frac{\partial \ln n_z}{\partial \theta} \right|^2 \sim \Delta^2 \sim \left| \frac{\partial \ln B}{\partial \theta} \right| \sim \epsilon \gg
\]

\[
\gg \left| \frac{\partial \ln n_e}{\partial \theta} \right| \sim \left| \frac{\partial \ln n_i}{\partial \theta} \right| \sim \frac{z_i e}{T_i} \left| \frac{\partial \Phi}{\partial \theta} \right| \sim \frac{z_i}{z} \left| \frac{\partial \ln n_z}{\partial \theta} \right|.
\] (5.5)

These orderings are in agreement with experimental observations (see the right hand-side of Fig. 1 of Ref. [20]) that show that the poloidal variation of the impurity density is significantly stronger than that of the magnetic field, radial electric field and impurity temperature. The latter is assumed to satisfy

\[
\frac{1}{\Delta^2} \left| \frac{\partial \ln T_z}{\partial \theta} \right| \ll 1.
\]

As a result, the weak poloidal variation of the impurity temperature can be ignored in the parallel impurity momentum equation.

5.2.3 Radial variation to retain diamagnetic flow effects

The characteristic length of the impurity density pedestal, \( L_{n_z} \), satisfies \( \rho_{pz} \ll L_{n_z} \ll \epsilon R \ll qR \). Here \( \rho_p = \frac{B}{H_p} \) is the poloidal (p) Larmor radius and \( qR \) is the connection length, with safety factor \( q \) and major radius \( R \). Consequently, the
impurity and bulk ion mean flows are taken to be slower than the thermal speed of the impurities [15,23,77].

The radial electric field on Alcator C-Mod is determined by combining the independently-measured impurity contributions to the perpendicular impurity momentum equation [29] to find

\[ E_r \approx \frac{1}{z_e n_z} \frac{\partial p_z}{\partial r} + V_{zt} B_p - V_{zp} B_t; \]  

(5.6)

where \( r \) is the radial coordinate, \( p \) the pressure, and \( V_t \) and \( V_p \) the toroidal (t) and poloidal (p) components of the mean flow. This equation provides strong motivation for retaining in H mode the impurity diamagnetic effect, \( \frac{1}{z_e n_z} \frac{\partial p_z}{\partial r} \), since experimental measurements (see Fig. 3 of Ref. [29], partially reproduced in Fig. 5.4) indicate that it can contribute more than 70% of the radial electric field in (5.6) for Boron. The \( E \times B \) and impurity diamagnetic effects are allowed to compete for the first time by ordering the impurity density radial variation to be stronger by a charge ratio than that of the potential and bulk ion density, leading to the following orderings for perpendicular gradients:

\[ \frac{1}{\rho_{pz}} \gg \frac{|\nabla \perp n_z|}{n_z} \sim \frac{z_z}{z_i} \frac{|\nabla \perp \Phi|}{T_i} \sim \frac{z_z}{z_i} \frac{|\nabla \perp n_i|}{n_i} \sim \frac{z_z}{z_i} \frac{|\nabla \perp T_i|}{T_i} \sim \frac{z_z}{z_i} \frac{|\nabla \perp T_z|}{T_z} \gg \frac{z_z}{z_i} \frac{|\nabla \perp B|}{B}; \]  

(5.7)

These orderings, schematized in Fig. 5.3, are in agreement with the experimental evidence in Fig. 5.1(b). Here the bulk ion temperature radial variation is taken to be as large as possible with the main ion diamagnetic effects competing but not overtaking the \( E \times B \) contribution. Given that equilibration forces \( T_i \sim T_z \) at all pedestal radial locations and that the radial variation of the impurity density is observed to be stronger than that of the impurity temperature (see right hand-side on Fig. 1 of Ref. [20]), it is reasonable to take the radial variation of both temperatures to be of the same order.

The experimental evidence of the importance of the diamagnetic effects is supported by theoretical evidence as well. By taking the radial derivative of
the Maxwell-Boltzmann bulk ion response and of the poloidally varying piece of quasineutrality, \( z_i (n_i - \langle n_i \rangle) - z_e (n_e - \langle n_e \rangle) \), a relationship between the radial variation of the poloidal part of the potential and the impurity and bulk ion densities consistent with (5.7) can be obtained:

\[
\frac{z_i n_{i}}{z_e n_{e}} \left( \frac{1}{T_i} + \frac{T_i}{z_e n_{i} n_{e}} \right) \frac{1}{n_{z}} \frac{\partial (n_{z} - \langle n_{z} \rangle)}{\partial \psi} = \frac{z_i e}{T_i} \frac{\partial (\Phi - \langle \Phi \rangle)}{\partial \psi} = - \frac{1}{n_{i}} \frac{\partial (n_{i} - \langle n_{i} \rangle)}{\partial \psi}.
\]  (5.8)

In summary, even though the poloidally dependent components of the potential and electron and bulk ion densities are much smaller than their corresponding flux surface averages (5.5), unlike in [15], the radial derivatives of these components
are allowed to compete since
\[
\frac{z_i}{z_e} \frac{\nabla \cdot (n_z - \langle n_z \rangle)}{n_z} \sim \frac{\nabla \cdot (\Phi - \langle \Phi \rangle)}{n_i} \sim \frac{\nabla \cdot (n_i - \langle n_i \rangle)}{n_i} \sim \frac{\nabla \cdot (n_e - \langle n_e \rangle)}{n_i}
\]
\[
\sim \frac{\Delta}{z_e} \frac{\nabla \cdot \langle n_z \rangle}{n_z} \sim \frac{\Delta}{n_i} \frac{\nabla \cdot \langle \Phi \rangle}{n_i} \sim \frac{\Delta}{n_i} \frac{\nabla \cdot \langle n_i \rangle}{n_i} \sim \frac{\Delta}{n_e} \frac{\nabla \cdot \langle n_e \rangle}{n_e}
\]
\[
\text{(5.9)}
\]

Since the negative slope of the impurity density is more negative on the inboard side (Fig. 5.1(b)), the model predicts via (5.9) the radial electric field be less negative on the inboard than on the outboard side. This is consistent with the experimental observation shown in Fig. 5.5.

### 5.2.4 Species collisionality

The assumptions of having lowest-order Maxwellian impurities, (5.7); bulk and impurity temperature equilibration, (7.15); banana regime, (5.12), Maxwell-Boltzmann
Figure 5.5: H-mode inboard and outboard radial electric field profiles when aligning the wells (adapted from Fig. 5 in [29]).

bulk ions, (5.13); and friction not affecting the lowest-order perpendicular impurity flow, (F.12), are checked a posteriori. These are the most restrictive inequalities and are obtained latter for the equation numbers given above. Doing so leads to the conclusion that self-consistency is satisfied when

\[
\min \left\{ 1, \sqrt{\frac{z_i L_{ns}}{z_z \rho_{pz}}} \right\} \gg \frac{\Delta z_i}{qR} \gg \max \left\{ \frac{\Delta z_z}{\varepsilon^2 \frac{z_z}{z_t}}, \frac{\rho_{pz}}{L_{ns}} \sqrt{\frac{z_z}{z_t}}, \frac{\rho_{pz}}{L_{ns}} \sqrt{\frac{z_z}{z_t}} \frac{B_{p}^2}{B_{t}^2} \right\}. \tag{5.10}
\]

Here \(\lambda\) is the mean free path, which is the thermal speed \(v_T = \sqrt{2T/M}\) divided by the sum of the like and unlike collision frequencies. Note also that the ratio of impurity to background ion mean free paths is given by

\[
\frac{\lambda_z}{\lambda_i} \sim \frac{\nu_{pz}}{\nu_{zi} + \nu_{tz}} \sim \left( \frac{z_i}{z_z} \right)^2, \tag{5.11}
\]

where \(z_{\text{eff}} \sim 1\) has been used to relate the collisional frequencies. In the collisional range under consideration (5.10), the self-collisional frequencies are much smaller.
than the gyrofrequency $\Omega = \frac{zeB}{cM} = \frac{v_T}{\rho}$, which is of the same order for main and impurity ions.

The assumptions of having lowest-order Maxwellian impurities and friction not affecting the lowest-order perpendicular impurity flow are checked in Appendices D and E, respectively. The bulk and impurity temperature equilibration is checked in Chapter 7.

The condition to have banana regime background ions,

$$\frac{qR}{\epsilon^2 \lambda_i} \ll 1,$$

could be rewritten by using (5.11) as a function of the impurity mean free path as follows:

$$\frac{\lambda_i}{qR \epsilon^2} \frac{z_i^2}{z_i^2} \gg 1. \quad (5.12)$$

The Maxwell-Boltzmann behaviour for the main ions is obtained if $T_i$ is a flux function and the bulk ion pressure and potential gradients are the dominant terms in the parallel momentum equation for the background ions, which requires

$$\frac{R_{iz}}{\nabla_i p_i + z_i e n_i \nabla_i \Phi} \sim \frac{\nu_i n_i M_i v_T z_i}{\Delta \frac{z_i p_i}{qR}} \sim \frac{1}{\Delta} \frac{qR \rho_{pz}}{\lambda_i L_{nz}} \left( \frac{z_i}{z_i^2} \right)^{\frac{3}{2}} \ll 1. \quad (5.13)$$
5.3 Impurity flow

This section is devoted to the calculation of the pedestal impurity flux including diamagnetic and non-diffusive radial flow effects self-consistently. To begin with, the perpendicular impurity flow is obtained from perpendicular momentum conservation for the impurities. Next, the impurity continuity equation is solved for the form of the parallel impurity flow within a flux function. The divergence of the radial flow has to be cleverly rearranged to facilitate the integration of the continuity equation. Finally, the parallel momentum equation for the impurities is considered and its solubility condition used to determine the unknown flux function. The friction with the background ions is modified due to retention of both the impurity diamagnetic flow and the radial flow effects that modify the the impurity parallel mean flow.

5.3.1 Perpendicular impurity flow

The momentum conservation for impurities balances electrostatic, magnetic, isotropic and anisotropic pressure forces, inertia and friction with the background:

\[
z_e e_n \left( \nabla \Phi - \frac{V_z \times B}{c} \right) + \nabla p_z + \nabla \cdot \pi_z + M_z n_z V_z \cdot \nabla V_z = R_{zi}. \tag{5.14}
\]

It is reasonable to assume that the perpendicular velocity is dominated by the \( E \times B \), as in \([15]\), and the new diamagnetic drift, since they are allowed to compete. The orderings (5.5), (5.7), (5.9) and (5.10) are chosen to make the perpendicular projection of the inertia, friction and divergence of the anisotropic pressure tensor negligible; as can be checked a posteriori in Appendix F. Therefore,

\[
V_{z \perp} = \frac{c}{B^2} B \times \left( \nabla \Phi + \frac{\nabla p_z}{z_e e_n z} \right) = \frac{c}{B^2} B \times \nabla \psi \left( \frac{\partial \Phi}{\partial \psi} + \frac{1}{z_e e_n z} \frac{\partial p_z}{\partial \psi} \right) + \frac{c}{B^2} B \times \nabla \theta \left( \frac{\partial \Phi}{\partial \theta} + \frac{1}{z_e e_n z} \frac{\partial p_z}{\partial \theta} \right). \tag{5.15}
\]
The axisymmetric tokamak magnetic field is taken to be
\[ B = I \nabla \zeta + \nabla \zeta \times \nabla \psi; \quad (5.16) \]
where \( \zeta \) is the toroidal angle, \( 2\pi \psi \) the poloidal magnetic flux with \( |\nabla \psi| = RB_p \) and \( I(\psi) = RB_1 \) a flux function. From (5.16), it follows that
\[ B \times \nabla \psi = IB - B^2 R^2 \nabla \zeta \quad (5.17) \]
and
\[ B \times \nabla \theta \cdot \nabla \psi = -IB \cdot \nabla \theta. \quad (5.18) \]

The projections of the perpendicular impurity mean flow (5.15) in the directions perpendicular to the flux surface (referred to as radial) and within the surface but perpendicular to the magnetic field are evaluated (5.18) to respectively find
\[ V_{z\perp} \cdot \nabla \psi RB_p = -\frac{c I B \cdot \nabla \theta}{B^2 RB_p} \left( \frac{\partial \Phi}{\partial \theta} + \frac{1}{z_z e n_z} \frac{\partial p_z}{\partial \theta} \right) \sim \frac{\rho_{pz} qR v_{Tz}}{\Delta \rho_{pz} qR v_{Tz}} \quad (5.19) \]
and
\[ \frac{V_{z\perp} \cdot B \times \nabla \psi}{BRB_p} = c \frac{RB_p}{B} \left( \frac{\partial \Phi}{\partial \psi} + \frac{1}{z_z e n_z} \frac{\partial p_z}{\partial \psi} \right) \sim \frac{\rho_{pz} qR v_{Tz}}{L_{nz}} \quad (5.20) \]
\[ + c \frac{\nabla \psi \cdot \nabla \theta}{BRB_p} \left( \frac{\partial \Phi}{\partial \theta} + \frac{1}{z_z e n_z} \frac{\partial p_z}{\partial \theta} \right) \sim s \Delta \rho_{pz} qR v_{Tz}. \]
The estimated size of the terms is shown to the right of the terms in (5.19) and (5.20), where \( s \) is the magnetic flux surface shape factor:
\[ 0 \lesssim s = r \nabla \theta \cdot \nabla \psi RB_p \lesssim 1. \quad (5.21) \]
Even though this factor is small in the concentric circle flux surface large aspect ratio limit, it is retained in this calculation for further accuracy.

### 5.3.2 Parallel impurity flow

The relationship between the perpendicular and parallel impurity flows must satisfy the conservation of particles equation,
\[ \nabla \cdot (n_z V_z) = \nabla \cdot (n_z V_{z\perp}) + B \cdot \nabla \left( V_{z\parallel} \frac{n_z}{B} \right) = 0. \quad (5.22) \]
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The divergence of the perpendicular flux in an axisymmetric tokamak is given by
\[ \nabla \cdot (n_z V_{\perp}) = B \cdot \nabla \left[ \frac{\partial}{\partial \psi} \left( \frac{n_z V_{\perp} \cdot \nabla \psi}{B \cdot \nabla \theta} \right) + \frac{\partial}{\partial \theta} \left( \frac{n_z V_{\perp} \cdot \nabla \theta}{B \cdot \nabla \theta} \right) \right]. \] (5.23)

The two components of the impurity flow, as given by (5.19) and (5.15), result in comparable contributions to the divergence when the impurity diamagnetic flow is retained as can be seen from
\[ \frac{\partial}{\partial \psi} \left( \frac{n_z V_{\perp} \cdot \nabla \psi}{B \cdot \nabla \theta} \right) \sim \frac{\partial}{\partial \theta} \left( \frac{n_z V_{\perp} \cdot \nabla \theta}{B \cdot \nabla \theta} \right) = \frac{eI}{z_e e B^2} \left( z_e e n_z \frac{\partial \Phi}{\partial \psi} + \frac{\partial p_z}{\partial \psi} \right). \] (5.24)

The preceding implies that the parallel dynamics depends on the perpendicular dynamics (Fig. 5.6(b)), in contrast to all the previous models [15] (Fig. 5.6(a)). In other words, the impurity radial flow affects the parallel flow when the diamagnetic flow is retained.

The physical phenomena included in the model, (5.4) and (5.5), have been purposely selected in order to make feasible the integration of the conservation of particles equation (5.22) to determine the impurity parallel flow. The first step towards expressing the divergence of the radial impurity flux (5.19) in the form of a parallel gradient of a scalar consists of using the relationships between the poloidal variation of the potential and impurity density in (5.4) to find
\[ \frac{\partial p_z}{\partial \theta} + z_e e n_z \frac{\partial \Phi}{\partial \theta} = \frac{\partial P}{\partial \theta} + O \left( \frac{\Delta^2}{z_z^2 p_z} \right); \] (5.25)

where
\[ P = (p_z - \langle p_z \rangle) + \frac{z_i^2 T_i}{z_i^2 n_i \left( 1 + \frac{n_e}{z_i n_i} \frac{T_i}{T_e} \right)} \left[ \langle n_z \rangle (n_z - \langle n_z \rangle) + \frac{(n_z - \langle n_z \rangle)^2}{2} \right]. \] (5.26)

Second, even though both impurity density and magnetic field poloidal variations are retained (5.5), their product \( \epsilon \Delta \) is assumed to be negligible, primarily to bring the magnetic field under the poloidal derivative to lowest order by writing
\[ \frac{I}{B^2} \frac{\partial P}{\partial \theta} = \frac{\partial}{\partial \theta} \left( \frac{IP}{\langle B^2 \rangle} \right) + \frac{I}{B^2} \left( 1 - \frac{B^2}{\langle B^2 \rangle} \right) \frac{\partial P}{\partial \theta} = \frac{\partial}{\partial \theta} \left( \frac{IP}{\langle B^2 \rangle} \right) + O \left( \frac{\epsilon \Delta I p_z}{B^2} \right). \] (5.27)
(a) Parallel dynamics can be individually analyzed in a one dimensional model without diamagnetic effects.

(b) Two dimensional effects given by the radial flow must be retained due to its large divergence to include impurity diamagnetic effects. Diamagnetic effects are included in the electric field, \( E_{\text{new}}^* = - (\nabla \Phi + \nabla_p \frac{v}{z e n_z}) \).

**Figure 5.6:** Schematic of the perpendicular impurity flow, given by the \( E \times B \) drift, that affects the parallel impurity flow in an tokamak cross section.

By using (5.19), (5.24), (5.25) and (5.27), the lowest order conservation of impurity particles equation (5.22) to order \( \epsilon \) can hence be rewritten as

\[
B \cdot \nabla \left[ \frac{n_z V_{\parallel}}{B} + \frac{c I}{z e B^2} \left( \frac{\partial p_z}{\partial \psi} + z e n_z \frac{\partial \Phi}{\partial \psi} \right) - \frac{c}{z e} \frac{\partial}{\partial \psi} \left( \frac{I P}{\langle B^2 \rangle} \right) \right] = 0. \tag{5.28}
\]

The parallel impurity flow is then obtained by integrating in poloidal angle to find

\[
V_{\parallel} = \frac{B K_z}{n_z} \frac{c I}{z e B n_z} \left( \frac{\partial p_z}{\partial \psi} + z e n_z \frac{\partial \Phi}{\partial \psi} \right) + \frac{c B}{z e n_z} \frac{\partial}{\partial \psi} \left( \frac{I P}{\langle B^2 \rangle} \right) \sim \rho_{p_z} \frac{v_{\parallel}}{L_{n_z}}, \tag{5.29}
\]

where \( K_z(\psi) \) is an unknown flux function. In conclusion, the impurity flow is given by

\[
V_z = V_{\perp z} + V_{\parallel} = B \left[ \frac{B K_z}{n_z} + \frac{c I}{z e B n_z} \left( \frac{I P}{\langle B^2 \rangle} \right) \right] - c R^2 \nabla \zeta \left( \frac{\partial \Phi}{\partial \psi} + \frac{1}{z e n_z} \frac{\partial p_z}{\partial \psi} \right)
+ \frac{c I}{B^2} \nabla \zeta \times \nabla \theta \left( \frac{\partial \Phi}{\partial \theta} + \frac{1}{z e n_z} \frac{\partial p_z}{\partial \theta} \right),
\tag{5.30}
\]

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where (5.16) and (5.17) have been used to evaluate the perpendicular impurity flow (5.15).

5.3.3 Calculation of the integration constant in the parallel impurity flow

Let us now turn our attention to the parallel impurity momentum conservation equation,

$$\nabla_{\parallel} p_z + z_z e_n z \nabla_{\parallel} \Phi + M_z n_z V_z \cdot \frac{B}{B} + \nabla \cdot \pi_{z} \cdot \frac{B}{B} = R_{zi\parallel}, \quad (5.31)$$

which is dominated by the friction and the impurity pressure and potential gradients. The inertial and diagonal (subscript $d$) and off-diagonal (subscript $g$) viscous forces can be neglected according to our orderings, since

$$\nabla \cdot \pi_{zdC} \cdot \frac{B}{B} \sim \frac{M_z n_z V_z \cdot \nabla_{\parallel} V_z}{\Delta \rho_{pz} L_{n_z}^2 q z q R} \sim \frac{M_z n_z \Delta \frac{\rho_{pz}}{q R} \frac{\rho_{pz}}{L_{n_z}}}{\Delta \rho_{pz} q R} \ll 1. \quad (5.32)$$

and

$$\nabla \cdot \pi_{zgC} \cdot \frac{B}{B} \sim \frac{M_z n_z V_z \cdot \nabla_{\parallel} V_z}{\Delta \lambda^2 \frac{\rho_{pz}}{q R} \frac{\rho_{pz}}{L_{n_z}} q R} \sim \frac{M_z n_z \Delta \frac{\rho_{pz}}{q R} \frac{\rho_{pz}}{L_{n_z}}}{\Delta \lambda^2 \frac{\rho_{pz}}{q R} \frac{\rho_{pz}}{L_{n_z}}} \ll 1. \quad (5.33)$$

Here the diagonal ($d$) and off-diagonal or gyroviscous ($g$) part of the viscous tensor are obtained on Eq. (42) and Eq. (44) of [78] (subscript $C$), respectively. The precise expressions can be found in Appendix E.1.2.

The calculation of the parallel friction force between impurities and the background ions, as outlined in Appendix C, leads to

$$R_{zi\parallel} = -\frac{\langle p_i \rangle}{\Omega_i} I_{t \nu_{iz}} \left[ \frac{d \ln \langle p_i \rangle}{d \psi} + z_i e d \langle \Phi \rangle \frac{3 d \ln T_i}{T_i d \psi} \right] + M_{i \nu_{iz}} \langle n_i \rangle \left( \frac{\langle n_i \rangle \ u B}{\langle n_i \rangle n_i} - V_{zi\parallel} \right). \quad (5.35)$$
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For banana main ions,

\[
\begin{align*}
\mu_i &= \frac{3\sqrt{2\pi}}{T_i^{3/2} M_i^{3/2}} \int \frac{d^3 v_i}{v_i^{3/2}} h_i \left( \psi, \frac{v_i}{v_i ||}, \mu_i = \frac{v_{i,\perp}}{2B}, E_i(\psi) = \frac{v_i^2}{2} + \frac{z_i e}{M_i} \langle \Phi \rangle \right)
\end{align*}
\]  

(5.36)

is a flux function since \( d^3 v_i \propto B v_i || \frac{d \mu_i}{d E_i(\psi)} \). Here \( h_i = f_i - f^{\dagger}_i M_i(\psi_i^*, E_i) \) vanishes in the trapped domain, where \( f_i \) is the main ion distribution function. The distribution \( f^{\dagger}_i M \) is a modification of a Maxwell-Boltzmann distribution depending only on the constants of the motion canonical angular momentum \( \psi_i^* = \psi - \frac{c_i M_i}{z_i e} \mathbf{R} \cdot \nabla \zeta \cdot v_i \), which replaces the \( \psi_i \) dependence, and total energy \( E_i = \frac{v_i^2}{2} + \frac{z_i e}{M_i} \Phi \).

The dominant terms in parallel momentum conservation, \( \nabla || p_z + z_i e n_z \nabla || \Phi = R_{z||} \), multiplied by the magnitude of the magnetic field can be evaluated by using (5.25) in the left hand side and (5.29) and (5.35) in the right hand side to find

\[
\mathbf{B} \cdot \nabla P = -M_i \left( \frac{n_z}{n_i} \right) \langle n_i \rangle \left[ \frac{cI}{z_i e} n_z T_i \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) - \frac{u B^2 n_z}{n_i} + B^2 K_z \right.
\]

\[
- \frac{cI}{z_i e} \frac{\partial p_z}{\partial \psi} - cI n_z \frac{\partial (\Phi - \langle \Phi \rangle)}{\partial \psi} + \frac{cB^2}{z_i e} \frac{\partial}{\partial \psi} \left( \frac{IP}{\langle B^2 \rangle} \right) \left. \right] \right.
\]

(5.37)

where the Coulomb logarithm has been taken to be a flux function.

The unknown flux function \( K_z \) in the parallel impurity flow (5.29) is determined by flux surface averaging the parallel momentum conservation (5.37), to find eventually that

\[
K_z = \frac{1}{\langle B^2 \rangle} \left[ \frac{cI}{z_i e} \frac{\partial \langle p_z \rangle}{\partial \psi} - \frac{cI}{z_i e} \langle n_z \rangle T_i \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) + \frac{u}{\langle n_i \rangle} \langle B^2 n_z \rangle + \frac{u}{\langle n_i \rangle} \langle B^2 n_z \rangle \right] .
\]

(5.38)

This form arises from the cancellation of terms justified as follows. The following term has been neglected in (5.38):

\[
- \frac{c}{z_i e} \left( \frac{B^2 - \langle B^2 \rangle}{\langle B^2 \rangle} \frac{\partial}{\partial \psi} \left[ \frac{IP - \langle P \rangle}{\langle B^2 \rangle} \right] \right) \sim \epsilon \Delta \ll 1,
\]

(5.39)

consistent with the orderings in (5.27). Also the non-linear terms cancel each other.

Silvia Espinosa Gútiez (sesp@mit.edu) 99/214
out to lowest order in (5.38),
\[
\frac{\partial \langle P \rangle}{\partial \psi} = \frac{z_e^2 T_i (n_z - \langle n_z \rangle) \partial (n_z - \langle n_z \rangle)}{z_i^2 \langle n_i \rangle \left(1 + \frac{n_i}{z_i n_i z_i T_i} \right)} = z_e e \left(\langle n_z - \langle n_z \rangle \rangle \frac{\partial (\Phi - \langle \Phi \rangle)}{\partial \psi} \right),
\]
\[ (5.40) \]
using the radial derivative of the flux surface average of (5.26), and (5.8). Finally, inserting the flux function (5.38) back into (5.30) and recalling that the radial variation of the magnetic field is negligible, the expression for the impurity flow when diamagnetic and radial flows are retained is obtained to be
\[
V_z = \frac{B}{n_z \langle B^2 \rangle} \left[ \frac{c I}{z_e} \frac{\partial \langle p_z \rangle + P}{\partial \psi} - \frac{c I}{z_i} \langle n_z \rangle T_i \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3 d \ln T_i}{2} \right) + \frac{u \langle B^2 n_z \rangle}{\langle n_i \rangle} \right]
- cR^2 \nabla \zeta \left( \frac{\partial \Phi}{\partial \psi} + \frac{1}{z_e n_z} \frac{\partial p_z}{\partial \psi} \right) + \frac{c I \langle B^2 \rangle \nabla \zeta}{\nabla \theta} \left( \frac{\partial \Phi}{\partial \theta} + \frac{1}{z_e n_z} \frac{\partial p_z}{\partial \theta} \right).
\]
\[ (5.41) \]
Notice that the last term has a radial component that is being retained.
5.4 Parallel momentum

The parallel momentum equation (5.37) can be further simplified by inserting \( K_z \) from (5.38) and neglecting the radial variation of the magnetic field and \( O(\epsilon \Delta) \) corrections to obtain

\[
\mathbf{B} \cdot \nabla P = -M_i \left\langle \frac{\nu_i}{n_z} \right\rangle \left\langle n_i \right\rangle \left\{ c I T_i \left\langle \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right\rangle \left( n_z - \frac{B^2}{\left\langle B^2 \right\rangle} \left\langle n_z \right\rangle \right) \\
- u B^2 \left( \frac{n_z}{\left\langle n_i \right\rangle} - \left\langle \frac{B^2}{\left\langle B^2 \right\rangle} \right\rangle \left\langle n_z \right\rangle \right) \\
- \frac{c I}{z_c e} \frac{\partial \langle p_z \rangle}{\partial \psi} \left( 1 - \frac{B^2}{\left\langle B^2 \right\rangle} \right) \\
+ \frac{c I}{z_c e} \frac{\partial [P - \langle p_z - \langle p_z \rangle \rangle]}{\partial \psi} - c I n_z \frac{\partial \langle \Phi - \langle \Phi \rangle \rangle}{\partial \psi} \right\}.
\] (5.42)

The left hand side can be evaluated to lowest order, by using (5.26) and recalling that the impurity density exhibits the strongest poloidal variation followed by the magnetic field, to find

\[
\frac{\partial P}{\partial \theta} = \langle T_z \rangle \frac{\partial (n_z - \left\langle n_z \right\rangle)}{\partial \theta} \left( 1 + \frac{z^2 \langle n_z \rangle}{z^2 \langle n_i \rangle} \right) \frac{T_i}{1 + \frac{\langle n_e \rangle \langle T_e \rangle}{z_i \langle n_i \rangle \langle T_i \rangle}} \left( n_z - \left\langle n_z \right\rangle \right) \frac{T_i}{\left\langle T_z \right\rangle} \left\langle n_z \right\rangle. \] (5.43)

Moreover, the dominant piece of the following term on the right hand side of (5.42) can be calculated by recalling that the impurity density exhibits both the strongest radial and poloidal variation and by using (5.8) as follows:

\[
\frac{\partial [P - \langle p_z - \langle p_z \rangle \rangle]}{\partial \psi} = \frac{z^2 T_i}{z^2 \langle n_i \rangle} \left( n_z \frac{\partial (n_z - \left\langle n_z \right\rangle)}{\partial \psi} + (n_z - \left\langle n_z \right\rangle) \frac{\partial \left\langle n_z \right\rangle}{\partial \psi} \right) \\
= z_c e n_z \frac{\partial \langle \Phi - \langle \Phi \rangle \rangle}{\partial \psi} + \frac{z^2 \langle n_z \rangle}{z^2 \langle n_i \rangle} \frac{T_i \left\langle n_z \right\rangle}{\left\langle T_z \right\rangle} \left( n_z - 1 \right) \frac{\partial \langle p_z \rangle}{\partial \psi}. \] (5.44)

The conservation of parallel momentum equation for impurities in dimensionless form is found by combining (5.42)-(5.44) to obtain

\[
(1 + \alpha n) \frac{\partial n}{\partial \theta} = g \left( n - b^2 \right) + U b^2 \left( n - \left\langle n b^2 \right\rangle \right) + D \left[ \alpha (n - 1) + b^2 - 1 \right] ; \] (5.45)
where the dimensionless density, \( n = \frac{n_x}{\langle n_x \rangle} \), and magnetic field squared, \( b^2 = \frac{B^2}{\langle B^2 \rangle} \), present strong poloidal variation which can be amplified by the following dimensionless flux functions

\[
\alpha = \frac{z_i^2(n_i)}{z_i^2(n_i) + \langle T_i \rangle \langle T_z \rangle z_i} \sim 1, \tag{5.46}
\]

\[
g = -\frac{cI}{z_i e} \langle B \cdot \nabla \theta \rangle \frac{\nu_{iz} T_i}{n_z} \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right), \tag{5.47}
\]

\[
U = \frac{u}{\langle T_z \rangle} \langle B \cdot \nabla \theta \rangle \nu_{iz} \frac{n_z}{\langle n_z \rangle} \tag{5.48}
\]

and

\[
D = -\frac{cI}{z_i e} \langle B \cdot \nabla \theta \rangle \frac{\nu_{iz}}{n_z} \frac{\partial \ln \langle p_z \rangle}{\partial \psi}. \tag{5.49}
\]

Note that when the impurity diamagnetic effects are neglected, by taking the \( D = 0 \) limit, Helander’s equation (9) in [15] is recovered.

The parallel momentum equation (5.45) can be further simplified by neglecting all \( O (\epsilon \Delta) \) corrections, to be consistent with previous assumption (5.27), to obtain

\[
(1 + \alpha n) \frac{\partial n}{\partial \theta} = g \left( n - b^2 \right) + U \left( n - 1 \right) + D \left[ \alpha (n - 1) + b^2 - 1 \right]
\]

\[
= (n - 1) \left( g + U + \alpha D \right) + (1 - b^2) \left( g - D \right) \tag{5.50}
\]
5.5 Discussion and conclusions

Improving the modeling of impurities is expected to yield deeper insight into how to avoid impurity accumulation and a better understanding and diagnostic methods for H (and I) mode operation in a tokamak. In this section the expressions for the various components of the impurity flow are extended to include the two-dimensional impurity diamagnetic are radial flow effects. These physical phenomena are shown here to obtain larger values of poloidal variation that the one-dimensional model [15], as observed. Finally, the novel expression for the impurity radial flux is derived and the diamagnetic effects are proven to beneficially enhance impurity removal, hence reducing or even preventing impurity accumulation while providing free fueling.

5.5.1 Poloidal impurity flow

The poloidal impurity flow has been experimentally observed (see Figs. 4.4, 4.5, 4.6 and 4.7 of [49]) to be much larger on the low field side of H-mode tokamak pedestals. The novel diamagnetic and radial effects included in the prior sections result in an additional term in the poloidal impurity flow (5.41),

\[
V_z \cdot \nabla \theta = \frac{B \cdot \nabla \theta}{n_z \langle B^2 \rangle} \left[ -\frac{cIT_i}{z_i e} \langle n_z \rangle \left( \frac{d \ln \langle p_i \rangle}{d\psi} - \frac{3}{2} \frac{d \ln T_i}{d\psi} \right) + u \frac{\langle B^2 n_z \rangle}{\langle n_i \rangle} + \frac{cI}{z_e e} \frac{\partial (p_z + P)}{\partial \psi} \right],
\]

(5.51)

with respect to the one-dimensional model [15].

\[
V_z \cdot \nabla \theta = \frac{B \cdot \nabla \theta}{n_z \langle B^2 \rangle} \left[ -\frac{cIT_i}{z_i e} \langle n_z \rangle \left( \frac{d \ln \langle p_i \rangle}{d\psi} - \frac{3}{2} \frac{d \ln T_i}{d\psi} \right) + u \frac{\langle B^2 n_z \rangle}{\langle n_i \rangle} \right].
\]

(5.52)

Both sources of poloidal variation are located out front of the square bracket in (5.52): the poloidal magnetic field, whose poloidal variation is weak in the large aspect ratio limit, and the inverse of the impurity density, which drives the poloidal
impurity flow to be significantly larger on the outboard as measured. The last term in (5.51), $\frac{\partial (p_z + P)}{\partial \psi}$, introduces poloidal variation within the square bracket.

The poloidal variation of the last term in (5.51) can be made more explicit by using (5.44) and recalling that the impurity density contains the strongest radial and poloidal variation, so that

$$\frac{\partial (p_z + P)}{\partial \psi} = \left( \langle T_z \rangle + \alpha T_i \frac{n_z}{\langle n_z \rangle} \right) \frac{\partial n_z}{\partial \psi} - \alpha T_i \frac{\partial \langle n_z \rangle}{\partial \psi}. \quad (5.53)$$

By substituting (5.53) into (5.51) and identifying the non-dimensional flux functions defined in (5.46)-(5.49), it is shown that the poloidal impurity flux over the poloidal magnetic field,

$$\frac{n_z \mathbf{V}_z \cdot \nabla \theta}{\mathbf{B} \cdot \nabla \theta} = \frac{\langle n_z \rangle \langle \mathbf{B} \cdot \nabla \theta \rangle}{\langle B^2 \rangle M_i \langle n_i \rangle^{\frac{\nu_d}{\nu_e}}} \left( g + U + \alpha D \right) + \frac{c I}{z_e e \langle B^2 \rangle} \left( 1 + \alpha \frac{T_i}{\langle T_z \rangle \langle n_z \rangle} \right) \frac{\partial n_z}{\partial \psi}, \quad (5.54)$$

is not a flux function in contrast to (15). The additional poloidal variation introduced by the diamagnetic and radial flow effects is given by the last term on the right hand side of (5.54). As Fig. 5.7 shows, the impurity density is larger on the high field side and its radial gradient is steeper (more negative) on the high field side. Therefore the final $(\frac{\partial n_z}{\partial \psi})$ term makes the poloidal flow asymmetry larger than previous models (15).
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It is worth noticing that the combination \( g + U + \alpha D \) in (5.54) must be positive when the poloidal flow is positive, since the second term in the right hand side of (5.54) is negative. In addition, by rewriting (5.53) as

\[
\frac{\partial (\langle p_z \rangle + P)}{\partial \psi} = [1 + \alpha (n-1)] \langle T_z \rangle \frac{\partial \langle n_z \rangle}{\partial \psi} + (1 + \alpha n) \langle T_z \rangle \frac{\partial (n_z - \langle n_z \rangle)}{\partial \psi},
\]

it is seen that this quantity is negative on the high field side for inboard accumulation and more negative inboard impurity density slope in agreement with H-mode experiments [20,29]. It thus follows from (5.51) that \( g + U \) should be positive for the poloidal flow to be positive on the high field side.

5.5.2 Parallel impurity flow

The parallel impurity flow has also been measured (see Figs. 4.4, 4.5, 4.6 and 4.7 of [49]) to be much larger on the outboard side of H-mode tokamak pedestals. The novel diamagnetic and radial effects and the stronger poloidal variation of the radial electric field included in the model also lead to an additional term in the parallel impurity flow (5.41),

\[
V_{z||} = - \frac{cI}{B} \frac{\partial \langle \Phi \rangle}{\partial \psi} + \frac{B}{n_z \langle B^2 \rangle} \left[ - \frac{cI}{z_i e} \langle n_z \rangle T_i \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) + u \frac{\langle B^2 n_z \rangle}{\langle n_i \rangle} \right]
+ \frac{cI}{z_z e n_z B} \left\{ \frac{B^2}{\langle B^2 \rangle} \frac{\partial (\langle p_z \rangle + P)}{\partial \psi} - \left[ \frac{\partial p_z}{\partial \psi} + z_z e n_z \frac{\partial (\Phi - \langle \Phi \rangle)}{\partial \psi} \right] \right\}, \tag{5.56}
\]

with respect to the one-dimensional model [15] which contains only the terms in the first line of (5.56). This term introduces a new source poloidal variation in addition to previous drives for the parallel impurity flow to be significantly larger on the low field side as experimentally observed, given by the inverse of the magnetic field on the first term in the first line of (5.56) and the poloidal variation of the inverse of the impurity density dominating that given by the magnetic field on the second term.

The term in (5.56) containing diamagnetic and radial flow effects and the
poloidal variation of the radial electric field is evaluated by using (5.44) to find
\[
\frac{B^2}{(B^2)} \frac{\partial}{\partial \psi} \left( \langle p_z \rangle + P \right) - \left[ \frac{\partial p_z}{\partial \psi} + z_z e n_z \frac{\partial (\Phi - \langle \Phi \rangle)}{\partial \psi} \right] = \\
= \frac{\partial \langle p_z \rangle}{\partial \psi} \left[ \left( \frac{B^2}{(B^2)} - 1 \right) + \alpha T_i \langle T_z \rangle \frac{n_z}{(n_z - 1)} \frac{B^2}{(B^2)} \right]; \quad (5.57)
\]
where to be consistent with (5.27) the following terms have been neglected:
\[
\left( \frac{B^2}{(B^2)} - 1 \right) \frac{\partial (p_z - \langle p_z \rangle)}{\partial \psi} \sim z_z e n_z \frac{\partial (\Phi - \langle \Phi \rangle)}{\partial \psi} \sim \epsilon \Delta \ll 1. \quad (5.58)
\]
From (5.57), it can be seen that the new term is negative on the high field side and positive on the low field side, since the impurity density is measured [20] to be larger on the high field side in H-mode. Consequently, the two-dimensional model with diamagnetic and radial effects that allows stronger poloidal variation of the radial electric field can capture substantially stronger in-out asymmetries in the positive parallel impurity flow than the previous state-of-the-art models [15].

5.5.3 Radial impurity particle flux

By taking the toroidal projection of impurity momentum conservation (5.14) and using axisymmetry, the radial particle flux is found to be
\[
n_z \textbf{V}_z \cdot \nabla \psi = \frac{c}{z_z e} R^2 \nabla \zeta \cdot \left( \textbf{R}_{iz} + M_z n_z \textbf{V}_z \cdot \nabla \textbf{V}_z + \nabla \cdot \pi_z \right). \quad (5.59)
\]
Using the estimates (5.32), (5.33), (5.34), (F.7), (F.12) and (F.21) to neglect small terms leads to the conclusion that friction dominates on the right hand side of (5.59), thus satisfying ambipolarity since
\[
z_z n_z \textbf{V}_z \cdot \nabla \psi = -\frac{c}{e} R^2 \nabla \zeta \cdot \textbf{R}_{iz} = -\frac{c}{e} R^2 \nabla \zeta \cdot \textbf{R}_{zi} \sim -z_i n_i \textbf{V}_i \cdot \nabla \psi. \quad (5.60)
\]
The calculation of the radial impurity particle flux can be further simplified by noticing that the parallel friction dominates since
\[
\frac{\textbf{R}_{iz \perp}}{\textbf{R}_{iz \parallel}} \cdot \frac{R \nabla \zeta}{R \nabla \zeta} = \frac{-\textbf{R}_{iz}}{\textbf{R}_{iz \parallel} \frac{1}{RB}} \sim \frac{B^2}{B^2} \ll 1, \quad (5.61)
\]
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where the estimate (F.10) has been used. As a result, the flux-surface averaged radial impurity particle flux is given to lowest order by

\[
\langle n_z V_z \cdot \nabla \psi \rangle = -\frac{cI}{z e \langle B^2 \rangle} \left( \frac{BR_{zi||}}{1 + (b^2 - 1)} \right)
\]

(5.62)

where in the last form the denominator has been Taylor expanded and the solubility constraint, \( \langle B R_{zi||} \rangle = 0 \), has been used. Finally, substituting the lowest order expression for the friction, whole poloidal variation is proportional to the right hand side of (5.50) divided by the magnetic field magnitude, the radial impurity flux becomes

\[
\langle n_z V_z \cdot \nabla \psi \rangle = -\frac{cI}{z e \langle B^2 \rangle} \left( \frac{BR_{zi||}}{1 - (b^2 - 1)^2} \right) \left( g + U + \alpha D \right) - \Delta \varepsilon^2 \frac{\rho z}{q R} n_z v_{Tz} R B_p ;
\]

Note that (13) in [15] is correctly recovered for \( D = 0 \) to lower order.

For illustrative purposes, a first-order cosinusoidal poloidal variation is considered for the dimensionless magnetic field, \( b^2 = 1 - 2\epsilon \cos \vartheta \), along with a first-order Fourier profile for the dimensionless impurity density, with both a cosinusoidal and sinusoidal term in order to allow for in-out and up-down asymmetries. It can then be observed that both of the flux surface averages on the right hand side of (5.63) are positive, since both the magnetic field and the impurity density are larger on the inboard than on the outboard. Since \( D \) is positive by definition and it is always proportional to a positive coefficient in (5.63), more impurities go out and ions go in as \( D \) increases. In conclusion, being in a regime with large diamagnetic drift helps to remove impurities.
Chapter 6

Addressing H-mode pedestal turbulence reduction concern: asymmetries captured

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6.1 Single sinusoid approximate solutions

The parallel momentum equation \( (5.50) \) can be linearized by neglecting the term of \( O(\alpha \Delta^2), \frac{\alpha}{2} \partial^2(n-1)/\partial \varphi^2 \), to find

\[
(1 + \alpha) \frac{\partial n}{\partial \varphi} = (n - 1)(g + U + \alpha D) + (1 - b^2)(g - D)
\]

(6.1)

For illustrative purposes, a first-order cosinusoidal profile is considered for the dimensionless magnetic fields squared, \( b^2 = 1 - 2\epsilon \cos \vartheta \), with \( \epsilon = \frac{1}{3} \); and a first-order Fourier profile for the dimensionless impurity density, \( n = 1 + C \cos \vartheta + S \sin \vartheta \), with both a sinusoidal and a cosinusoidal term in order to allow for up-down and in-out asymmetries respectively. Note that \( \alpha C^2 \ll 1 \), \( \alpha S^2 \ll 1 \) and \( \alpha CS \ll 1 \) for the linear model to apply.

Substituting these poloidal profiles in (6.1) and separating the cosinusoidal and sinusoidal dependences lead to the following system of equations:

\[
S (1 + \alpha) = C (g + U + \alpha D) + 2\epsilon (g - D)
\]

\[
-C (1 + \alpha) = S (g + U + \alpha D)
\]

The impurity density in-out and up-down poloidal variations are thus given by

\[
C = \frac{-2\epsilon (g - D)(g + U + \alpha D)}{(1 + \alpha)^2 + (g + U + \alpha D)^2}
\]

(6.2)

and

\[
S = \frac{2\epsilon (g - D)(1 + \alpha)}{(1 + \alpha)^2 + (g + U + \alpha D)^2},
\]

(6.3)

respectively.

In this chapter, the maximum impurity density in-out asymmetry that the model with impurity diamagnetic and radial flow effects can capture is analyzed. Attention is drawn to the significant improvements in performance and robustness when compared to previous models \(^{15}\). Figure 6.1 shows the impurity density
Figure 6.1: Impurity density in-out asymmetry factor, $\frac{n_{IN}}{n_{OUT}} = \frac{1-C}{1+C}$, as a function of the dimensionless ‘impurity diamagnetic’ friction parameter, $D$. Each curve corresponds to particular values of effective impurity charge $\alpha$, ‘bulk ion diamagnetic’ $g$ and ‘kinetic’ friction $U$; distinguished by symbol filling, shape and color respectively. The experimental value of a six fold inboard impurity concentration [20] is indicated by a dotted line. The closest value in each curve to the experimental one is circled.

in-out asymmetry, $\frac{n_{IN}}{n_{OUT}} = \frac{1-C}{1+C}$, as a function of the dimensionless ‘impurity diamagnetic’ friction parameter, $D$; for representative combinations of effective impurity charge $\alpha$, ‘bulk ion diamagnetic’ $g$ and ‘kinetic’ friction $U$ values. Note that the previous one-dimensional models [15] without impurity diamagnetic effects, $D = 0$, correspond to the vertical axis.

The maximum in-out asymmetry can be found where its first derivative with respect to the impurity diamagnetic effects vanishes with a negative second derivative, as analytically calculated in Sec. 6.4 and illustrated by the dark green and red
circled curves in the upper left of Fig. 6.1. However, one should bear in mind that the maximum in-out asymmetry can also be reached at a physical boundary for the impurity diamagnetic flow and impurity density, as explained and analytically calculated in Sec. 6.2. The first type of physical boundary is given by the value at $D = 0$, where the maximum is reached for instance in the light and dark blue curves in Fig. 6.1. The second type is given by the impurity density becoming negative at some poloidal angle, where the maximum in-out asymmetry is reached for example in the dark purple diamonds and light green and red circles curves in the upper left of Fig. 6.1. Finally, the maximum in-out asymmetry can rarely be reached for an unphysically large value of the dimensionless impurity diamagnetic friction, such as in the light purple curve in the lower right of Fig. 6.1. This limit is analytically calculated in Sec. 6.3.

6.2 Physical constraints on allowable parameters

6.2.1 Physical impurity diamagnetic flow and proper reduction to previous models

The dimensionless impurity diamagnetic flow parameter $D$ must also be non-negative by definition [5.49], $D \geq 0$. The associated physical boundary is thus given by $D = 0$ (subscript $D$), which corresponds to the previous one-dimensional models with neither impurity diamagnetic nor radial flow effects [2,3,15]. In this limit, the impurity density in-out (6.2) and up-down (6.3) asymmetry coefficients properly reduce to

$$C_D = \frac{-2\epsilon g (g + U)}{(1 + \alpha)^2 + (g + U)^2}$$

(6.4)
and

\[ S_{B'} = \frac{2\epsilon g (1 + \alpha)}{(1 + \alpha)^2 + (g + U)^2}, \]  

(6.5)

respectively.

### 6.2.2 Physical impurity density: non-negative density at all angles

In addition to the physical boundary without impurity diamagnetic effects, given by \( D = 0 \), the impurity density must be non-negative at all poloidal angles by definition. This is obtained when

\[ C^2 + S^2 \leq 1; \]  

(6.6)

since

\[ n = C \cos \vartheta + S \sin \vartheta = \sqrt{C^2 + S^2} (\cos \psi \cos \vartheta + \sin \psi \sin \vartheta) = \sqrt{C^2 + S^2} \cos (\vartheta - \psi) \]  

(6.7)

where \( \tan \psi = \frac{S}{C} \).

- **Without impurity diamagnetic effects:**

  The impurity density in-out (6.4) and up-down (6.5) asymmetry coefficients must satisfy

  \[ C_B^2 + S_B^2 = \frac{(2\epsilon)^2 g^2}{(1 + \alpha)^2 + (g + U)^2} \leq 1 \]  

  (6.8)

  in order to have an impurity density physically possible.

- **With impurity diamagnetic effects:**
The limit where the impurity density becomes zero at some poloidal angle, given by \( C^2 + S^2 = 1 \), can also be expressed as a function of physical quantities like \( D \), \( g \) and \( U \). Actually, the latter condition can be expressed by using (6.2) and (6.3) as the following second order equation in \( D \):

\[
D^2 \left[ (2\epsilon)^2 - \alpha^2 \right] - 2D \left[ g \left( (2\epsilon)^2 + \alpha (g+U) \right) \right] + \\
+ \left[ g^2 (2\epsilon)^2 - (1+\alpha)^2 - (g+U)^2 \right] = 0. \tag{6.9}
\]

Each solution constitutes a new physical boundary only for positive values of \( D \). Here the physical values of impurity diamagnetic flow \( D \) where the impurity density becomes zero at some poloidal angle are identified from the non-physical ones. The entire range of positive and negative bulk ion fluid \( g \) and kinetics \( U \) effects and non-negative effective impurity charge \( \alpha \) are considered.

To begin with, the case when \( \alpha = 2\epsilon \) is analyzed separately since (6.9) becomes a first order equation,

\[
D = \frac{g^2 (2\epsilon)^2 - (1 + 2\epsilon)^2 - (g+U)^2}{4\epsilon \left[ g (1+2\epsilon) + U \right]}. \tag{6.10}
\]

The range of \( g \) and \( U \) when this solution is non-negative are analytically derived in Appendix H.1.1 and summarized in Table H.1.

In summary, when \( \alpha = 2\epsilon \) there is a boundary of the physical region given by (6.10) in the following regions:

- If \( g \leq -\frac{1+\alpha}{2\epsilon} \), then when

\[
U < -g - \sqrt{g^2 (2\epsilon)^2 - (1 + 2\epsilon)^2}
\]

or

\[
-g + \sqrt{g^2 (2\epsilon)^2 - (1 + 2\epsilon)^2} < U \leq -g (1 + 2\epsilon).
\]

- If \( -\frac{1+\alpha}{2\epsilon} < g \leq \frac{1+\alpha}{2\epsilon} \), then when

\[
U \leq -g (1 + 2\epsilon).
\]
CHAPTER 6. IMPURITY DENSITY IN-OUT ASYMMETRIES CAPTURED

- If \( \frac{1 + \alpha}{2\epsilon} < g \), then when
  
  \[
  U \leq -g (1 + 2\epsilon)
  \]
  
  or
  
  \[
  -g - \sqrt{g^2 (2\epsilon)^2 - (1 + 2\epsilon)^2} < U < -g + \sqrt{g^2 (2\epsilon)^2 - (1 + 2\epsilon)^2}.
  \]

For \( \alpha \neq 2\epsilon \), the second order equation in (6.9) is solved for the dimensionless impurity diamagnetic effects to find

\[
D = \frac{g (2\epsilon)^2 + \alpha (g + U)}{(2\epsilon)^2 - \alpha^2}
\]

\[
\pm \sqrt{[g (2\epsilon)^2 + \alpha (g + U)]^2 - [(2\epsilon)^2 - \alpha^2] [g^2 (2\epsilon)^2 - (1 + \alpha)^2 - (g + U)^2]}
\]

\[
(2\epsilon)^2 - \alpha^2
\]

(6.11)

This expression can be simplified to obtain, after some algebra,

\[
D = \frac{g (2\epsilon)^2 + \alpha (g + U) \pm \sqrt{(2\epsilon)^2 [g (1 + \alpha) + U]^2 + [(2\epsilon)^2 - \alpha^2] (1 + \alpha)^2}}{(2\epsilon)^2 - \alpha^2}
\]

(6.12)

In Appendix H.1.2, the physical domain in \( \alpha, g \) and \( U \) space for which any or both of the solutions for \( D \) are non-negative are analytically derived in detail. The results are summarized here in Table H.2.

In summary, when \( \alpha < 2\epsilon \) there is a boundary of the physical region in the following regions:

- If \( g \leq -\frac{1 + \alpha}{2\epsilon} \), then the ‘+’ root, corresponding to the ‘+’ sign in (6.11) or (6.12), is positive when
  
  \[
  U < -g - \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}
  \]
  
  or
  
  \[
  U > -g + \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}.
  \]

- If \( -\frac{1 + \alpha}{2\epsilon} < g \leq \frac{1 + \alpha}{2\epsilon} \), then the ‘+’ root of (6.11) or (6.12) is always positive.
If \( \frac{1+\alpha}{2\epsilon} < g \), then the ‘+’ root of (6.11) or (6.12) is always positive. The ‘−’ root of (6.11) or (6.12) is also positive only when

\[
-g - \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2} < U < -g + \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}.
\]

When \( \alpha > 2\epsilon \) there is a boundary of the physical region in the following regions:

- If \( g \leq \frac{-\alpha (1+\alpha)}{2\sqrt{\alpha^2 - (2\epsilon)^2}} \), then the ‘+’ root of (6.11) or (6.12) is positive when

\[
U < -g - \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}
\]

while the ‘−’ root is positive when

\[
U < -g + \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}.
\]

- If \( \frac{-\alpha (1+\alpha)}{2\sqrt{\alpha^2 - (2\epsilon)^2}} < g \leq \frac{1+\alpha}{2\epsilon} \), then the ‘+’ root of (6.11) or (6.12) is positive when

\[
U < -g - \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}
\]

or

\[
-g + \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2} < U \leq (1 + \alpha) \left[ -g - \frac{\alpha^2 - (2\epsilon)^2}{2\epsilon} \right]
\]

while the ‘−’ root is positive when

\[
U \leq (1 + \alpha) \left[ -g - \frac{\alpha^2 - (2\epsilon)^2}{2\epsilon} \right].
\]

- If \( \frac{1+\alpha}{2\epsilon} < g \leq \frac{1+\alpha}{2\epsilon} \), then both the ‘+’ and ‘−’ roots of (6.11) or (6.12) are positive when

\[
U \leq (1 + \alpha) \left[ -g - \frac{\alpha^2 - (2\epsilon)^2}{2\epsilon} \right].
\]
 CHAPTER 6. IMPURITY DENSITY IN-OUT ASYMMETRIES CAPTURED

- If $\frac{1+\alpha}{2\epsilon} < g \leq \frac{\alpha(1+\alpha)}{2\epsilon\sqrt{\alpha^2-(2\epsilon)^2}}$, then the ‘+’ root of (6.11) or (6.12) is positive when

$$U \leq (1 + \alpha) \left[ -g - \frac{\sqrt{\alpha^2 - (2\epsilon)^2}}{2\epsilon} \right]$$

while the ‘−’ root is positive when

$$U \leq (1 + \alpha) \left[ -g - \frac{\sqrt{\alpha^2 - (2\epsilon)^2}}{2\epsilon} \right]$$

or

$$-g - \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2} < U < -g + \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}.$$

- If $\frac{\alpha(1+\alpha)}{2\epsilon\sqrt{\alpha^2-(2\epsilon)^2}} < g$, then the ‘+’ root of (6.11) or (6.12) is positive when

$$U \leq (1 + \alpha) \left[ -g - \frac{\sqrt{\alpha^2 - (2\epsilon)^2}}{2\epsilon} \right]$$

or

$$(1 + \alpha) \left[ -g + \frac{\sqrt{\alpha^2 - (2\epsilon)^2}}{2\epsilon} \right] \leq U < -g - \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}.$$

while the ‘−’ root is positive when

$$U \leq (1 + \alpha) \left[ -g - \frac{\sqrt{\alpha^2 - (2\epsilon)^2}}{2\epsilon} \right]$$

or

$$(1 + \alpha) \left[ -g + \frac{\sqrt{\alpha^2 - (2\epsilon)^2}}{2\epsilon} \right] \leq U < -g + \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2}.$$

6.3 Strong impurity pressure radial variation

For large dimensionless impurity diamagnetic flow parameter $D$, the impurity density in-out and up-down asymmetry coefficients are given by

$$\lim_{D \to +\infty} C = \frac{2\epsilon}{\alpha} \geq 0$$  \hspace{1cm} (6.13)

and

$$\lim_{D \to +\infty} S = 0^-.$$  \hspace{1cm} (6.14)
respectfully. Note that $2\epsilon \leq \alpha$ is a necessary condition for the $C$ limit to be physical.

## 6.4 Maximum in-out asymmetry with diamagnetic flow effects

There is an extremum in the impurity density in-out asymmetry, $\frac{\partial C}{\partial D} = 0$, when the following values of the dimensionless diamagnetic effects

$$D_{\pm} = \frac{1}{\alpha} \left[ -\frac{(1 + \alpha)^2}{g(1 + \alpha) + U} - (g + U) \pm (1 + \alpha) \sqrt{1 + \left( \frac{1 + \alpha}{g(1 + \alpha) + U} \right)^2} \right]$$

are physical, i.e. both its value and the corresponding impurity density at all poloidal angles are non-negative.

The maximum in-out asymmetry corresponding to inboard accumulation is given by the minimum value of the in-out asymmetry coefficient $C$, a.k.a. the negative value with the largest magnitude. The value of (6.15) that additionally satisfies

$$\frac{\partial^2 C}{\partial D^2} > 0$$

is

$$D = \begin{cases} D_- & \text{if } g(1 + \alpha) + U < 0 \\ D_+ & \text{if } g(1 + \alpha) + U > 0 \end{cases}$$

(6.16)

This value is continuous at the boundary, $g(1 + \alpha) + U$, since

$$\lim_{g(1+\alpha)+U \to 0^-} D_- = g$$

(6.17)

and

$$\lim_{g(1+\alpha)+U \to 0^+} D_+ = g.$$  

(6.18)
Due to the fact that the value of $D$ corresponding to a maximum impurity density in-out asymmetry is monotonously decreasing and goes from $-\infty$ to $+\infty$, as proven in Appendix I, there is one and only one value of $U$ where $D = 0$. Depending on $g$, the root is given by

$$\begin{cases} D_- [U = U^*] = 0, & \text{if } g < 0, \\ D [U = 0] = 0, & \text{if } g = 0, \\ D_+ [U = U^*] = 0, & \text{if } g > 0; \end{cases}$$

where $U^*$ is obtained to be

$$U^* = \frac{1}{3} \left[ - (3 + \alpha) g + \frac{-3(1+\alpha)^2 + (\alpha g)^2}{\sqrt{\text{disc}}} + \frac{3}{\sqrt{\text{disc}} \sqrt{1 + \alpha}} \right]$$

with

$$\text{disc} = 18\alpha g (1 + \alpha)^2 - (\alpha g)^3 +$$

$$+ 3\sqrt{3} (1 + \alpha) \sqrt{(1 + \alpha)^4 + 11 (\alpha g)^2 (1 + \alpha)^2 - (\alpha g)^4}. \quad (6.21)$$

Recall that only the places where $D \geq 0$, corresponding to $U \leq U^*$, are physically meaningful.

### 6.5 Parameter-space survey with diamagnetic effects

In this section, attention is drawn to the differences in impurity density in-out asymmetry with respect to previous theories [15]. An example is illustrated in Fig. 6.2, which shows the impurity density in-out asymmetry as a function of the impurity diamagnetic effects for three representative combinations of kinetic $U$ and fluid bulk ion friction $g$ and effective impurity charge $\alpha$ values. The effective charge of $\alpha = 0.25$ is used in all curves since is the closest to the expected value for Boron...
CHAPTER 6. IMPURITY DENSITY IN-OUT ASYMMETRIES CAPTURED

Figure 6.2: Improvement with respect to previous models [15] in robustly capturing experimental impurity density in-out asymmetries.

(see Sec. 3.2). The impurity-ion friction can be divided into three components whose relative size is given by $g$ for the ‘bulk ion diamagnetic’ friction, $U$ for the ‘kinetic’ friction and $D$ for the ‘impurity diamagnetic’ friction. The main difference between the curves is the relative bulk ion density slope with respect to that of the bulk ion temperature in $g$. This value is chosen to be positive in all the cases, as generically observed in H-mode [19]. The experimental value of a six fold inboard impurity concentration [20] is indicated by a dashed grey line. The H-mode pedestal has been observed to be in the plateau regime [24]. Kinetic theory with trace impurities associates this collisionality regime with a negative value of $U$. A value of $U \approx -2.0$ is selected for all the curves, making small adjustments to capture the experimental value of 6. The in-out asymmetry predicted by the one-dimensional models [15] without impurity diamagnetic effects corresponds to
the value at the vertical axis where $D = 0$, as highlighted in a black box in Fig. 6.3.

To begin with, for the blue-squared curve in Fig. 6.2, which corresponds to an intermediate $g$, the one-dimensional model predicts an outboard impurity accumulation contradicting the experiments. The present model with two-dimensional impurity diamagnetic and radial flow effects instead predicts inboard impurity accumulation. For the purple shaded circles curve, which corresponds to the bulk ion temperature being half as steep as the bulk ion density ($g = 0.0$), the new model can lead to substantially larger in-out asymmetries than the one-dimensional model and reaches experimental value of six for a physically reasonable value of the impurity diamagnetic effects. In the case with magenta diamonds, which corresponds to a clearly dominant bulk ion density gradient with respect to the temperature one, the impurity density is not even physical without impurity diamagnetic effects for some cases such as, for instance, the parameters corresponding to the magenta-diamond curve; since it becomes negative at some poloidal angle. However, this effect is a consequence of the approximations in the present calculation and does not occur for the full solution of Helander’s equations; see Sec. 6.7.

Contours of impurity density in-out asymmetry are used from now on in order to analyze the whole domain in kinetic $U$ and fluid bulk ion friction $g$ and effective impurity charge $\alpha$ space. As illustrated in Fig. 6.3, blue is used for outboard impurity accumulation in contradiction with the experiments, while red is used for the experimentally observed six-fold inboard impurity accumulation. The intermediate color used is yellow, since white is reserved to denote the unphysical regions, given by a non-positive impurity density at some poloidal angle. Apart from the contour color corresponding to the one-dimensional model result, attention is drawn as well to the impurity density in-out asymmetry that is the closest to the six that the two-dimensional model can obtain. This maximum in-out asymmetry for a given set of $\alpha$, $g$ and $U$ values is indicated in Fig. 6.3 with a
Figure 6.3: Illustration of the impurity density in-out asymmetry contour legend. The outboard impurity accumulation is indicated in blue while the experimental six fold value of inboard impurity accumulation or larger is indicated in red. The intermediate color is chosen to be yellow instead of white, since the latter is reserved for non-physical values. Finally, the previous models [15], which correspond to the vertical axis where $D = 0$, are highlighted in a black rectangle.

circle. For instance, the corresponding contour where the circle is located is green for the blue-squared curve, while red for the other two curves.

Slices at constant measurable effective impurity charge are presented. The impurity density in-out asymmetry predicted by the state-of-the-art one-dimensional models [15] can be calculated by using (6.4) to find the contours in Fig. 6.4. Physical boundaries can be given by the impurity density becoming negative at some poloidal angle. The impurity diamagnetic flow that corresponds to the maximum in-out asymmetry can be found at a physical boundary or where the first derivative
of the latter vanishes with a negative second derivative, as analytically calculated in Sec. 6.2 and Sec. 6.4, respectively. Note that the red bottom left diagonal parameter region implies impurity poloidal flow in contradiction with experimental observations, as will be proven later in Chapter 7.

Fig. 6.5 shows the contours of strictly positive ‘impurity diamagnetic’ friction corresponding to the closest in-out asymmetry to six, which is represented in Fig. 6.6. As highlighted by a black circle in Fig. 6.1, this closest value to the experimental one can be found at a maximum or a physical boundary. The contours of impurity density up-down asymmetry corresponding to the maximum impurity density in-out asymmetry is given in Fig. 6.7. In that figure, blue indicates lower impurity accumulation, while the rest upper impurity accumulation.

The maximum impurity density in-out asymmetry allowed by the two-dimensional model with radial and impurity diamagnetic effects is compared side by side with that predicted by the one-dimensional model in Fig. 6.4. Particular attention is drawn to the effective charge of 0.25 in Fig. 6.8, since it is the closest to the expected value for Boron (see 3.2).

In the upper part of Fig. 6.8, it can be observed that the one-dimensional model [15] can only capture the experimental six-fold inboard impurity accumulation in red for large $g$ in magnitude, $|g| \gtrsim 3$. Both of the regions where the experimental values are captured are right next to a white unphysical region, where the density becomes negative at some poloidal angle. The two-dimensional model developed captures the experimental value for all sizes of the ‘bulk ion diamagnetic’ friction $g$ in the lower part of Fig. 6.8.
Figure 6.4: Contours of impurity density in-out asymmetry obtained without diamagnetic effects [15].
Figure 6.5: Contours of dimensionless ‘impurity diamagnetic’ friction $D$ corresponding to the closest impurity density in-out asymmetry to the experimental value [20], as a function of effective impurity charge $\alpha$, ‘bulk ion diamagnetic’ $g$ and ‘kinetic’ $U$ friction.
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Figure 6.6: Contours of impurity density in-out asymmetry for the dimensionless ‘impurity diamagnetic’ friction $D$ in Fig. 6.5. In other words, contours of the in-out asymmetry closest to the experiment that the two-dimensional model can capture.
Figure 6.7: Contours of impurity density up-down asymmetry for the dimensionless ‘impurity diamagnetic’ friction $D$ in Fig. 6.6. Blue indicates lower impurity accumulation, while the rest upper impurity accumulation.
Figure 6.8: Comparison of the contours of impurity density in-out asymmetry without ‘impurity diamagnetic’ friction (up) and with the optimal dimensionless ‘impurity diamagnetic’ friction $D$ (down) for $\alpha = 0.25$. 
CHAPTER 6. IMPURITY DENSITY IN-OUT ASYMMETRIES CAPTURED

(a) Impurity density up-down asymmetry.  
(b) Impurity density in-out asymmetry.

Figure 6.9: Contours for the dimensionless ‘impurity diamagnetic’ friction $D$ in Fig. 6.5.  
A representative point of each of the regions exhibiting the experimental in-out impurity density asymmetry has been marked.

The three-dimensional plots containing the whole domain in kinetic $U$ and fluid $g$ bulk ion friction and effective impurity charge $\alpha$ variables are relegated Appendix J.

Fig. 6.10(a) shows the polar plots for the dimensionless impurity density correspondent to two sets of ‘kinetic’ and ‘bulk ion diamagnetic’ friction values that represents each of regions where the in-out asymmetry value of six is predicted.  
Fig. 6.9(a) and 6.9(b) highlight their exact location in the impurity density up-down and in-out asymmetry contours, respectively. The purple and green crosses are located at $g = -3.0$ and $g = 3.0$, both with $U = -1.0$.  In the polar plot in Fig. 6.10(a) the dimensionless impurity density magnitude is given by the radius while the angle represents the angle in the tokamak, whose cross section is sketched in Fig. 6.10(b).  In Fig. 6.10(a) it can be seen that the regions on the right and left of Fig. 6.9(b) correspond to upper and lower impurity accumulation, respectively.

The two-dimensional model with impurity diamagnetic and radial effects developed allows stronger density in-out asymmetries than prior theories.
(a) Dimensionless impurity density polar plots for the representative points marked in Fig. 6.9 with a purple $(g = -3.0)$ and green $(g = 3.0)$ cross respectively both with $U = -1.0$.

Figure 6.10: Dimensionless impurity density polar plots for the representative points marked in Fig. 6.9. Here the angle is the tokamak angle in Fig. 6.10(b) while the radius the magnitude.

6.6 Non-linear numeric solutions

The impurity parallel momentum equation can be solved iteratively if the non-linear term was retained:

$$\alpha n \frac{\partial n}{\partial \vartheta} + (g + U + \alpha D) + (b^2 - 1) (g - D) = -\frac{\partial n}{\partial \vartheta} + n (g + U + \alpha D) \quad (6.22)$$

Note that this conservation equation has been rearranged with this purpose in mind by gathering the terms containing the first power of the impurity density on the right hand side, while keeping the non-linear term calculated from the value
The impurity density profile is represented by using a complete Fourier series,

\[ n = \sum_{j=-N}^{j=N} n_j e^{ij\vartheta}, \]  

that is truncated at \( N = 15 \) since the results are independent of \( N \) from then on.

The cosinusoidal profile for the magnetic field can be easily expressed in that base to find

\[ b^2 = 1 - 2\epsilon \cos \vartheta = -\epsilon e^{-i\vartheta} + 1 - \epsilon e^{i\vartheta}. \]  

This non-linear numeric analysis is used to show the approximations effects of the linear single-mode analysis previously provided in this chapter. Fig. 6.11 presents the non-linear numerical solutions corresponding to the illustrative parameters chosen in Fig. 6.2. It can be observed that the values computed non-
linearly are close to the ones calculated by analytically solving the linear equation, plotted with empty and filled symbols respectively. The difference between them decreases as the impurity density in-out asymmetry gets smaller, from less than 5% for a six fold in the shaded magenta diamond and purple circle curves to completely negligible in the blue square curve. Most importantly, the solutions are also qualitative similar with the prediction of a non-physical impurity density when using the model without radial and impurity diamagnetic effects for the parameters corresponding to the magenta diamond curve. At those regions, the models break down due to the assumption $\epsilon (n - 1) \ll 1$. Consequently, the single-mode analytical linear calculations performed in this chapter are quantitatively sufficiently accurate. In addition, the equations found provide insight on the physical phenomena that increase the impurity density in-out asymmetry and reduce the non-physical regions.

6.7 Non-linear parallel momentum equation
including the $\epsilon (n - 1)$ terms

Equation (5.50) differs even when $D = 0$ from the parallel momentum equation of Helander [15] which is

$$
(1 + \alpha n) \frac{\partial n}{\partial \vartheta} = g (n - b^2) + Ub^2 \left( n - \langle nb^2 \rangle \right).
$$

The differences consist in that (5.50) has dropped terms of order $\epsilon (n - 1)$ in the $U$ coefficient because terms of that order are omitted in the two-dimensional calculation of the coefficient of $D$. It turns out that this omission of one-dimensional terms causes negative density solutions that are avoided by equation (6.25).

Therefore in this section we explore the solution of equations retaining the full one-dimensional expressions. This is justified if the diamagnetic parameter $D$ is
in which the $D$ terms are not necessarily accurate to $O[\epsilon (n - 1)]$, because of the terms of the form $DO[\epsilon (n - 1)]$ that were neglected in order to perform the integral of the conservation of impurity particles. This non-linear equation is solved iteratively, by calculating the left hand side using the impurity density from the previous iteration and then solving for the new impurity density via matrix inversion.

Fig. 6.12 compares the non-linear numerical solutions with the linear ones, plotted with empty and filled symbols respectively, corresponding to the illustrative linear analytical results (filled symbols) in Fig. 6.2.

![Figure 6.12: Validation via non-linear numeric solutions (empty symbols) of the comprehensive and illustrative linear analytical results (filled symbols) in Fig. 6.2](image-url)
Figure 6.13: Effect of the ‘kinetic’ friction on the impurity density in-out asymmetry for constant values of $g$ and $\alpha = 0.25$. This corresponds to vertical lines in the contours previously shown, but solving (5.43) for convergence. The impurity density in-out asymmetries with and without ‘impurity diamagnetic’ friction are represented in the upper axis in light and dark blue lines, respectively. The optimal dimensionless ‘impurity diamagnetic’ friction is used to calculate the latter and plotted in the lower axis in green symbols.
It can be observed that, while the impurity density in-out asymmetry is over predicted by the linear solution for the magenta diamond curve, the values computed non-linearly for the blue square and purple circle curves are very close to the ones calculated by analytically solving the linear equation, except for the span of the unphysical regions. The most substantial difference is actually the impurity density, with neither impurity diamagnetic nor radial effects, remaining positive for all the cases for the non-linear equation.

The fact that the solutions without impurity diamagnetic effects are always physical for \( g > 0 \) can be seen clearly in Fig. 6.13. This corresponds to vertical lines in contours like those on Fig. 6.4 since constant values of \( g \) and \( \alpha = 0.25 \) are used. The impurity density in-out asymmetries with and without ‘impurity diamagnetic’ friction are represented in the upper axis in light and dark blue lines, respectively. The optimal dimensionless ‘impurity diamagnetic’ friction used to calculate the latter is plotted in the lower axis in green symbols. Apart from observing that the solution without impurity diamagnetic and radial flow effects in light blue is physical in the whole domain where \( g > 0 \) where the equation converges, one can see that the two-dimensional model in dark blue significantly increases the impurity density in-out asymmetry in the area where \( g + U \) is negative.

The effect of the impurity diamagnetic effects on the dimensionless impurity density polar plots obtained by iteratively solving the non-linear impurity parallel momentum conservation (5.45) is illustrated in Fig. 6.14 for a cosinusoidal magnetic field with \( \epsilon = \frac{1}{3} \). Detailed data regarding the parameters used, minimum dimensionless impurity density and in-out asymmetry factor for each of the curves in Fig. 6.14 are provided in Table 6.1. The parameters used in Fig. 6.14(a) correspond to the magenta diamond curve in Fig. 6.2 in order to illustrate the non-linear term making the impurity density non-negative even without impurity diamagnetic effects. Fig. 6.14(b) has the same parameters as the purple circle curve in Fig. 6.2 except for an almost negligible increase in \( g \) that leads to an out-
(a) $U = -1.6$, $g = 3.0$ and $\alpha = 0.25$.

(b) $U = -2.1$, $g = 0.0^+$ and $\alpha = 0.25$.

**Figure 6.14:** Effect of the impurity diamagnetic effects on the dimensionless impurity density polar plots obtained by iteratively solving the non-linear impurity parallel momentum conservation (6.22) for a cosinusoidal magnetic field with $\epsilon = \frac{1}{3}$. Parameters correspond to the magenta diamond (a) and purple circle (b) curves in Fig. 6.2.

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**Table 6.1:** Impurity density in-out asymmetry factor for the profiles in Fig. 6.14
board impurity accumulation when impurity diamagnetic effects are not included. Fig. 6.14(b) and the corresponding dimensionless impurity density in-out asymmetry values shown in Table 6.1 illustrate that the impurity diamagnetic effects can correctly predict inboard impurity accumulation significantly larger than in the one-dimensional model.
Chapter 7

Impurity temperature poloidal variation and experimental comparison


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7.1 Introduction

We now analyze the impurity energy equation, and find that compressional heating can cause a difference $T_z - T_i$ between impurity and bulk ion temperatures. This difference is proportional to the product $(g + U + \alpha D) \frac{\partial n_z}{\partial \vartheta}$ (7.13); so it depends upon the impurity density poloidal asymmetry, and particularly the in-out variation of $T_z - T_i$ depends on the up-down impurity density asymmetry. But also its sign depends on the sign of $(g + U + \alpha D)$. This combination of coefficients also determines the sign of the poloidal impurity flow (5.54).

The state-of-the-art neoclassical models [2,3,15,23–27] assume impurities in thermal equilibrium with weakly poloidally varying background ions. In this chapter, the impurity temperature poloidal variation driven by the compressional heating in the energy equation is calculated in Sec. 7.2. Then, the simultaneous features of impurity density and temperature in-out asymmetry are analyzed in Sec. 7.3. Insight into pedestal profile alignment is also provided.

7.2 Temperature poloidal variation from energy equation

The impurity energy equation balances convection, compressional heating, viscous energy, the divergence of the conductive heat flux, $q_z$ and equilibration,

$$\frac{3}{2} n_z \mathbf{V}_z \cdot \nabla T_z + p_z \mathbf{V}_z \cdot \nabla \mathbf{V}_z + \pi_z : \nabla \mathbf{V}_z + \nabla \cdot q_z = \frac{3}{2} \nu_z n_z (T_i - T_z). \quad (7.1)$$

This equation justifies taking the bulk ion temperature to be a lowest order flux function, since it is not measured at two poloidal locations and the left hand side of (7.1) can drive the poloidal variation of the impurity temperature. I have found the orderings for the left hand side to be dominated by compressional heating,
which prevents complete equilibration by introducing poloidal dependence that drives the impurity temperature away from the poloidally independent bulk ion temperature. The remaining terms are all small since

$$\frac{3}{2} n_z V_z \cdot \nabla T_z \sim \max \left\{ \frac{1}{\Delta} \frac{\partial \ln T_z}{\partial \theta} , \frac{z_i}{z} \right\} \ll 1,$$

(7.2)

$$\frac{\pi_{adC}}{p_z \nabla \cdot V_z} \sim \max \left\{ \frac{\rho_{pz}}{L_{nz}} \frac{\Delta}{q R} , \frac{\Delta}{q R^2} \frac{\partial \ln T_z}{\partial \theta} , \left( \frac{\rho_{pz}}{q R} \frac{\partial \ln T_z}{\partial \theta} \right)^2 \right\} \ll 1,$$

(7.3)

$$\frac{\pi_{gC}}{p_z \nabla \cdot V_z} \sim \max \left\{ \frac{z_i}{z} , \frac{1}{\Delta} \frac{\partial \ln T_z}{\partial \theta} , \frac{\Delta}{q R} \frac{\rho_{pz}}{L_{nz}} \frac{\partial \ln T_z}{\partial \theta} \right\} \ll 1,$$

(7.4)

and

$$\frac{\nabla \cdot q_{RC}}{p_z \nabla \cdot V_z} \sim \max \left\{ \frac{z_i}{z} , \frac{1}{\Delta} \frac{\partial \ln T_z}{\partial \theta} , \frac{\Delta}{q R} \frac{\rho_{pz}}{L_{nz}} \frac{\partial \ln T_z}{\partial \theta} \right\} \ll 1.$$

(7.5)

The compressional heating can be rewritten by using conservation of impurity particles as

$$p_z \nabla \cdot V_z = - T_z \cdot \nabla n_z.$$

(7.6)

Importantly, even when the radial component of the impurity flow (5.19) is very small with respect to the poloidal impurity flow (5.20, 5.29),

$$V_{z \perp} \cdot B \nabla \psi_{BRB} \sim \frac{V_{z \perp} \cdot B \nabla \psi_{BRB}}{\Delta L_{nz} \epsilon R} \ll 1,$$

(7.7)

the radial variation of the impurity density is strong enough, recall (5.5), that its divergence can compete with the divergence of the poloidal flow. This implies that both components of the perpendicular impurity flow must be retained in the conservation equations when the impurity flow is dotted into a gradient of the impurity density since

$$V_z \cdot \nabla \ln n_z \sim V_{z \perp} \cdot \nabla \psi_{BRB} \frac{\partial \ln n_z}{\partial \psi} \sim V_z \cdot \nabla \theta \frac{\partial \ln n_z}{\partial \theta} \sim \Delta \frac{\rho_{pz}}{L_{nz}} \frac{v_{rz}}{q R}.$$

(7.8)

The compressional heating can then be evaluated from the poloidal and radial impurity flow (5.41) using axisymmetry, where $O(\epsilon \Delta)$ corrections can be
neglected, to obtain

$$\mathbf{V}_z \cdot \nabla n_z = \frac{\mathbf{B} \cdot \nabla \theta}{n_z \langle B^2 \rangle} \frac{\partial n_z}{\partial \theta} \langle n_z \rangle \left[ - \frac{c I T_i}{z_i e} \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) + \frac{u \langle B^2 \rangle}{\langle n_i \rangle} \right]$$

$$+ \frac{\mathbf{B} \cdot \nabla \theta}{n_z \langle B^2 \rangle} \frac{c I}{z_i e} \left[ \frac{\partial n_z}{\partial \theta} \frac{\partial (\langle p_z \rangle + P)}{\partial \psi} - \frac{\partial n_z}{\partial \psi} \left( z_z e n_z \frac{\partial \Phi}{\partial \theta} + \frac{\partial p_z}{\partial \theta} \right) \right].$$

(7.9)

This expression can be further simplified by using (5.44) and recalling that the impurity density exhibits the strongest radial and poloidal variations to obtain

$$\frac{\partial (\langle p_z \rangle + P)}{\partial \psi} = \langle T_z \rangle \frac{\partial n_z}{\partial \psi} + \alpha T_i \left( \frac{n_z}{\langle n_z \rangle} \frac{\partial n_z}{\partial \psi} - \frac{\partial \langle n_z \rangle}{\partial \psi} \right).$$

(7.10)

In addition, by recalling (5.25) and (5.43), the radial flow can be evaluated to find

$$z_z e n_z \frac{\partial \Phi}{\partial \theta} + \frac{\partial p_z}{\partial \theta} = \frac{\partial P}{\partial \theta} = \frac{\partial n_z}{\partial \theta} \left( \langle T_z \rangle + \alpha T_i \frac{n_z}{\langle n_z \rangle} \right).$$

(7.11)

All the terms in (7.10) and (7.11) but one cancel when they are inserted into (7.9).

The resulting expression for the compressional heating is thus

$$p_z \nabla \cdot \mathbf{V}_z = -T_z \mathbf{V}_z \cdot \nabla n_z =$$

$$= T_z \frac{\mathbf{B} \cdot \nabla \theta}{n_z \langle B^2 \rangle} \frac{\partial n_z}{\partial \theta} \langle n_z \rangle \left[ \frac{c I T_i}{z_i e} \left( \frac{d \ln \langle p_i \rangle}{d \psi} - \frac{3}{2} \frac{d \ln T_i}{d \psi} \right) - \frac{u \langle B^2 \rangle}{\langle n_i \rangle} \right]$$

$$+ \frac{c I}{z_i e} \left( \langle T_z \rangle \frac{\partial \ln \langle n_z \rangle}{\partial \psi} \frac{T_i}{\langle T_z \rangle} \right).$$

(7.12)

In conclusion, energy balance between compressional heating and equilibration therefore reduces to

$$\frac{T_z - T_i}{T_z} = \frac{\langle B \cdot \nabla \theta \rangle^2}{\langle B^2 \rangle} \langle T_z \rangle \left( g + \alpha D \right) \frac{1}{n^2} \frac{\partial n}{\partial \theta}.$$  

(7.13)

where $2M_in_i \nu_{zi} = M_z n_z \nu_{zi}$ is used along with the bulk ion density being a flux function to lowest order. The previous expression is valid in the comprehensive impurity collisionality regime specified in (5.10). When the friction is taken to compete with the pressure and potential gradient terms in parallel momentum conservation, then the equilibration term dominates the energy equation since

$$\frac{2^{-\frac{1}{2}} \nu_{zi} (T_z - T_i)}{v_{\parallel}} \sim \Delta \lambda_R \sqrt{\frac{z_i \nu_{zi}}{\nu_{zi} \nu_{z}} L_{ns}} \sim \left( \frac{\rho_{pz}}{L_{ns}} \right)^2 \ll 1.$$  

(7.14)
CHAPTER 7. IMPURITY TEMPERATURE POLOIDAL VARIATION

The impurity temperature is then equal to lowest order to the bulk ion temperature, which is taken to be a flux function. The poloidal variation of the impurity temperature can then be related to that of the impurity density and its poloidal derivative by using \( T_z \approx T_i \) in the terms in (7.13) that do not contain the difference to conclude

\[
\frac{T_z}{T_i} - 1 = \frac{4 \langle B \cdot \nabla \theta \rangle^2 T_i}{3 \langle B^2 \rangle \langle \nu_{zi} \rangle^2 M_z} (g + U + \alpha D) \frac{1}{n^2} \frac{\partial n}{\partial \theta} \sim \Delta \frac{\lambda_z}{q R} \sqrt{\frac{z_z}{\rho_{pz}}} L_{ns}. \tag{7.15}
\]

The success of the model developed in simultaneously obtaining both the experimentally observed six-fold inboard impurity accumulation and a larger outboard impurity temperature is proven in Sec. 7.3.1. Moreover, the prediction of the model regarding the impurity density up-down asymmetry is shown to be also in agreement with experimental observations in Sec. 7.3.2.

7.3 Validation of the model predictions against experimental evidence

7.3.1 Impurity density and temperature in-out asymmetries

experimental values captured

It can be deduced from (7.13) that the poloidal derivative of the inverse of the impurity density drives the impurity temperature away from a flux function. Furthermore, when considering a first-order Fourier profile for the dimensionless impurity density as in Chapter 6, it can be observed that it is the up-down asymmetry of the impurity density that drives the impurity temperature in-out asymmetry.

The flux function \( \sigma = \frac{4 \langle B \cdot \nabla \theta \rangle^2 T_i}{3 \langle B^2 \rangle \langle \nu_{zi} \rangle^2 M_z} \) in (7.13) is positive by definition. Hence, the direction of the impurity temperature in-out asymmetry depends on the impurity density up-down asymmetry and the sign of \( g + U + \alpha D \). It has been indicated where this latter quantity changes its sign in the impurity density up-down and
CHAPTER 7. IMPURITY TEMPERATURE POLOIDAL VARIATION

(a) Impurity density up-down asymmetry.  
(b) Impurity density in-out asymmetry.

Figure 7.1: Impurity density up-down and in-out asymmetry contours for the dimensionless ‘impurity diamagnetic’ friction $D$ plotted in Fig. 6.5. The dashed black line, $g + U + \alpha D = 0$, indicates negligible impurity temperature poloidal variation according to (7.13). A representative point of each of the regions exhibiting the experimental in-out impurity density asymmetry have been marked with an x in purple and green for the $g + U + \alpha D < 0$ and $g + U + \alpha D > 0$ region, respectively. Finally, the regions not shadowed in purple exhibit larger outboard impurity temperature, as experimentally observed.

in-out asymmetry contours in Fig. 7.1 by a dashed black line. By using the sign of $g + U + \alpha D$ and the impurity density up-down asymmetry in Fig. 7.1(a) in (7.13), the region with larger inboard impurity temperature has been shadowed in purple in order to leave visible only the region whose impurity temperature is in qualitative agreement with the experimental observations. It can be observed in Fig. 7.1(b) that both of the regions in red where the experimental six-fold impurity accumulation are captured lead to a larger outboard temperature in agreement with the observed values [20].

Figure 7.2 shows the dimensionless impurity density temperature polar plots, in solid and dashed lines respectively, for the representative points marked in each of the red regions where the experimental in-out asymmetry values are captured. The region represented by the purple marker in Fig. 7.1 has a negative $g+U+\alpha D$, which
CHAPTER 7. IMPURITY TEMPERATURE POLOIDAL VARIATION

(a) \( g + U + \alpha D < 0 \).

(b) \( g + U + \alpha D > 0 \).

Figure 7.2: Dimensionless impurity density (solid) temperature (dashed) polar plots for the representative points marked in Fig. 7.1. Here the angle is the tokamak angle while the radius the magnitude. From the illustrative values of \( \sigma = \frac{4 \langle B \cdot \nabla \theta \rangle^2 T_i}{3 \langle B^2 \rangle \langle \nu_z \rangle^2 M_z} \) selected to calculate the impurity temperature from (7.13), the long dashed value leads simultaneously to the experimentally observed impurity temperature and density in-out asymmetry.

corresponds to impurity accumulation below the equatorial plane in Fig. 7.2(a).

In contrast, the region represented by the green marker in Fig. 7.1 has a positive \( g + U + \alpha D \), which corresponds to impurity accumulation above the equatorial plane in Fig. 7.2(b). Importantly, note that the experimentally observed six-fold inboard impurity accumulation and outboard impurity temperature 25% larger than the inboard one are simultaneously captured in Fig. 7.2(a) and 7.2(b) for \( \sigma = 0.02 \).
7.3.2 Poloidal impurity flux and impurity density up-down asymmetry

In the previous subsection, the sign of $g + U + \alpha D$ has been proven to determine if there is upper or lower impurity accumulation. In this subsection, it is discovered that some direct experimental measurements can be used to determine its sign.

In particular, recall that the variable $g + U + \alpha D$ appears in the definition of the poloidal impurity flow in (5.54),

$$\frac{n_z V_z \cdot \nabla \theta}{B \cdot \nabla \theta} = \frac{\langle n_z \rangle \langle B \cdot \nabla \theta \rangle}{\langle B^2 \rangle M_i \langle n_i \rangle \langle \nu_{\perp} / n_z \rangle} (g + U + \alpha D) + \frac{c I}{\beta_e \langle B^2 \rangle} \left( 1 + \alpha \frac{T_i}{T_e} \frac{n_z}{\langle n_z \rangle} \right) \frac{\partial n_z}{\partial \psi} \quad (7.16)$$
(a) Impurity density up-down asymmetry.  

(b) Impurity density in-out asymmetry.

**Figure 7.4:** Similar to Fig. 7.1 but shading away in dark purple the area whose poloidal impurity flux direction contradicts the experimental evidence presented in Fig. 7.3.

The poloidal impurity flow can be measured via charge exchange recombination spectroscopy. For instance, Fig. 7.3 shows the inboard (HFS) and outboard (LFS) radial profiles of the boron poloidal flow in Alcator C-Mod for different types of H-modes. First, it can be observed that the poloidal flow is larger on the outboard side in the pedestal region across the board. Second, the poloidal flow is in the same direction as the magnetic field and thus positive with both the experimental and theoretical sign conventions for all the H-mode types under study in Fig. 7.3. Consequently, the left hand side of (5.54), which is reproduced in (7.16) for convenience of the readers, is positive. Since the second term on the right hand side of (5.54) is negative due to the radial derivative, the first term on the right hand and thus \( g + U + \alpha D \) must be positive.

The impurity density up-down and in-out asymmetry contours in Fig. 7.4 are similar to those in Fig. 7.1 but shading in dark purple indicates the area whose poloidal impurity flux direction contradicts the experimental evidence presented in Fig. 7.3. As a consequence, the area consistent with the experimental data from charge exchange recombination spectroscopy is represented by the polar profiles in Fig. 7.2(b) with positive poloidal flow and thus upper impurity accumulation. This upper impurity accumulation prediction is in agreement with Alcator C-Mod.
vertical emission profile measurements shown in Fig. 7.5

7.3.3 Insight on pedestal profile alignment

The fact that this section has shown that the impurity temperature can vary in a flux surface weakens any argument that the experimental ambiguity in flux-surface location should be resolved by assuming the impurity temperature to be a flux function. It is noted also that the two-dimensional theory includes non-zero terms of the form $\frac{\partial(\Phi - \Phi_i)}{\partial \phi}$, which correspond to poloidal variations of the radial electric field and weaken arguments for ‘$E_r$-alignment’ [20]. If the coefficients of the present theory $(g + U + \alpha D)$ were known experimentally from poloidal flow the $T_z - T_i$ would be deducible.
Chapter 8

Conclusions

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8.1 Overall summary and conclusions

In summary, in this thesis research I devise a neoclassical impurity radial flux measuring method \cite{2,3} from diagnostics currently available, providing insight on optimal tokamak operation to actively prevent impurity accumulation. It predicts outward neoclassical impurity flux occurs for I-mode operation in C-Mod; making the presence of the sometimes undetected weakly coherent mode unnecessary to explain its properties. This is consistent with the $\mathbf{E} \times \mathbf{B}$ flow shear observed in both I and H-mode regimes, which may break up eddies to reduce the turbulence level leading to good bulk energy confinement.

Measurements during the last decade of stronger poloidal asymmetries than predicted by the most comprehensive neoclassical models put into question either this turbulence reduction in H-mode pedestals or the physical phenomena included in neoclassical models. I have developed a self-consistent theoretical model retaining the experimentally observed impurity diamagnetic flow and the challenging two-dimensional features that it implies due to its associated non-negligible radial flow divergence. This two dimensional nonlocal feature is missing in all previous models, even those claiming to treat impurity diamagnetic effects. It successfully captures simultaneously the experimental impurity density, temperature and radial electric field in-out asymmetries for physical values of the impurity diamagnetic effects; thus making them consistent with H-mode pedestal turbulence reduction. Furthermore, not only can the poloidal variations obtained for the impurity temperature be used to align the outboard and inboard radial profiles, but also the expressions for the impurity flow and conservation equations may improve our ability to model pedestals and literally bring existing codes \cite{44,45} to a new dimension.
8.2 Part I: Pedestal radial flux measuring method and theoretical explanation of I-mode impurity removal

In the first part of the thesis, I provide a practical way of evaluating the pedestal radial flux for non-trace impurities from measurements currently available. One of its main advantages is that it conveniently bypasses the computationally demanding kinetic calculation of the full bulk ion response, by using the solubility constraint to express the latter in terms of the poloidal impurity flow.

The neoclassical radial impurity flux has two components. The direction of the first is shown to be related to the impurity in-out asymmetry and the poloidal flow direction, both obtainable via change-exchange recombination spectroscopy. Inboard impurity accumulation with poloidal flow in the direction of the magnetic field or outboard impurity accumulation with opposite poloidal flow direction are desirable. The direction of the second term depends on the relative slope of the main ion density and temperature profiles, which can be estimated by those of electrons and impurities and thus measured by Thomson scattering and charge-exchange spectroscopy respectively. A bulk ion temperature profile more than twice as steep as the density is shown to lead to impurity removal and fuel absorption by this term.

The proposed measuring method can be used to optimize tokamak operation to reduce if not prevent impurity accumulation while providing natural fueling. For instance, toroidal rotation and ICRF minority heating can be used to push impurities outwards or inwards respectively. Moreover, peeling-balloning mode excitation \cite{57} and scrape-of-layer high density reduction \cite{50,53} via impurity seeding \cite{54} can lead to a stronger and weaker radial variation of the electron temperature and density, respectively. Including these effects for highly-charged
impurities motivates generalizing the illustrative large aspect ratio results presented in Chapter 2 to allow for large flows in general tokamak cross sections with realistic aspect ratio in Chapter 3, including also an arbitrary poloidal electric field modeling the effect of additional species and plasma heating.

In Chapter 4, the direction of the neoclassical radial impurity flux in I-mode is evaluated for highly-charged impurities, based on recent experimental data and the radial impurity flux measuring method presented in previous chapters. An inward neoclassical radial impurity flux would make turbulence solely responsible for pushing impurities out. However, I find that the neoclassical theory correctly predicts an outward radial impurity flux, without the need of invoking anomalous mechanisms. Thus, I-mode operation with impurity removal and good energy confinement is allowed to occur when the weakly coherent mode is not detected in agreement with observations. Furthermore, I propose a new criterion to distinguish H-mode and I-mode based on the direction of the neoclassical radial impurity flux, being inwards for the former and outwards for the latter. Finally, my work suggests that the presence of strong $E \times B$ shear may explain the high energy accumulation observed in both modes, due to the decorrelation of the turbulence and its reduction.

8.3 Part II: Theoretical explanation of pedestal poloidal variation, addressing the concern regarding H-mode pedestal turbulence reduction

In Chapter 5, I propose that the impurity diamagnetic drift, which has been measured to be of the same order as the ExB drift, is a key physical phenomenon that pedestal neoclassical models were missing. Retaining it captures the unexpectedly strong poloidal variation observed experimentally, and hence finally address the
concern regarding turbulence reduction in H-mode pedestals of the last decade.

Importantly, I have proven that radial flow effects must be retained in order to include impurity diamagnetic effects, since the radial gradients of the impurity density must be allowed to be stronger by the charge ratio that that of the bulk ion density for not so highly-charged impurities. I have developed a self-consistent two-dimensional theoretical neoclassical model for axisymmetric tokamak pedestals. In contrast to all the previous models [2,3,15,23,27], including those claiming to include impurity diamagnetic effects [33], the impurity parallel dynamics is here affected not only by flows contained in the flux surface but also by the impurity radial flows out of the flux surface. The novel expressions for the impurity flow and conservation equations may improve our ability to model pedestals and extend existing codes to a new dimension.

In Chapter 6, the experimental six-fold inboard accumulation, with impurity poloidal flow in the direction of the magnetic field, is obtained even with the one-dimensional model for values consistent with physical constraints in contradiction to previous papers claims [24]. Moreover, the two-dimensional model with impurity diamagnetic and radial effects developed can more robustly capture substantially stronger density in-out asymmetries than the state-of-the-art models, especially in the region where the impurity poloidal flow goes in the opposite direction than the magnetic field. The new phenomenon acts as an amplification factor on the magnetic field poloidal variation drive.

In Chapter 7, I devise the self-consistent orderings that allow the compressional heating to prevent complete temperature equilibration between impurities and the main ions, resulting in the first to my knowledge neoclassical model with impurity temperature poloidal variation.

It explains collisionally the experimental impurity density, temperature and radial electric field in-out asymmetries; thus making them consistent with H-mode pedestal turbulence reduction. The two-dimensional model developed with impu-
ritiy diamagnetic and radial flow effects is shown to simultaneously capture the experimental values of impurity temperature and density in-out asymmetry. Furthermore, the direction of the radial electric field in-out asymmetry and impurity density up-down asymmetry are also accurately predicted. Having addressed the H-mode pedestal turbulence reduction concerns, the poloidal profiles of the impurity temperature that this model provides allow also the alignment of inboard and outboard radial profiles as a bonus.

8.4 Impact on future research

8.4.1 Theoretical fusion community

This theoretical thesis provides insight into I and H-mode impurity transport and energy confinement. The outward collisional impurity flux found allows for I-mode impurity removal to occur when the weakly coherent mode is not detected, in agreement with experimental observations. The presence of strong $E \times B$ shear is proposed to explain the good energy confinement observed in both modes, due to turbulence reduction. The latter in H-mode pedestal is shown consistent with strong experimental poloidal variation. This consistency is confirmed by developing a neoclassical model with radial flow affecting the parallel dynamics, which self-consistently includes impurity diamagnetic effects in agreement with the experimental evidence.

This new model has been developed for flows slower than the impurity thermal velocity, in agreement with experimental observations. For flows of the order of the impurity thermal velocity, both inertia and gyroviscosity would affect the parallel momentum equation when retaining diamagnetic effects. The available expressions for the viscous tensor are now affected by the presence of non-trace impurities. In addition, the collision operator is modified for these large flows, as
CHAPTER 8. CONCLUSIONS

shown in Appendix G.

8.4.2 Experimental fusion community

The method of measuring the radial impurity flux from available diagnostics discussed here is aimed at guiding experimental efforts to prevent impurity accumulation and thus improve fusion performance to a commercial level in several tokamaks around the world, such as Alcator C-Mod, ASDEX-Upgrade, JET and DIII-D. Thomson scattering and charge exchange spectroscopy units are already installed and currently allow the calculation of radial fluxes of typical impurities such as boron, carbon and nitrogen. Not only the performance of different types of modes and operation regimes with respect to preventing impurity accumulation can now be assessed by measuring the radial impurity flux, but also the suggestions regarding actively reducing impurity accumulation via neutral beam injection, ion cyclotron resonance heating and impurity seeding could be put into practice both individually and simultaneously.

The calculated poloidal variation of the impurity temperature could be used not only to align the profiles but also to decide the diagnostics placement, by choosing the regions of lower or higher temperature to protect the equipment or amplify the emission respectively. This work leads us to suggest the addition of charge spectroscopy exchange units to the top and bottom of the tokamak, in addition to those on the high and low field side. This would provide a check in addition to that provided by the impurity in-out asymmetries for the predictions of the model with radial and impurity diamagnetic flow effects. In addition, the measurements of the components of the impurity-ion friction, and thus the predicted impurity density in-out asymmetry, become more and more accurate with the improvement of the pedestal diagnostics, as the error bars associated become smaller. Finally, in the long run, when the diagnostics have improved enough, the analysis of the response of really highly charged impurity, such as tungsten or molybdenum, would make a
great contribution towards a better understanding of the mechanism for impurity removal and natural fueling.

### 8.4.3 Computational fusion community

The results in this thesis could have an impact on the computational fusion community. First, the proposed new method of solving the neoclassical equations not only makes codes faster but it also makes them significantly more accurate. Indeed, the achievement of bypassing the computationally demanding calculation of the background ion kinetic response also eliminates errors associated with the simplifying assumptions that codes have to make to make this calculation tractable; such as, those coming from neglecting poloidal variation. Even though it is bypassed, if this kinetic calculation could eventually be done in the future with the retention of poloidal variation as codes evolve, it could be used to self-consistently complete all the impurity neoclassical models.

Second, the expressions for the conservation equations and the impurity flow presented in the second part of the thesis are currently being implemented in several pedestal codes, since they literally open a new dimension that could be further characterized in the future. Pedestal modelling in substantially better agreement with the experiments may also lead to a superior tokamak design.
Appendix A

Thesis structure
### Table A.1: Thesis structure, including the main characteristics of the theoretical model of each of the parts, the main idea and result, chapters contained and patents \(^1\) and publications \(^2\)–\(^7\) corresponding to each of them.

<table>
<thead>
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<th>Main idea and result</th>
<th>Model and meaning</th>
<th>Chapter</th>
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<td>1D Independent</td>
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<td>(^1) (^2)</td>
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<td>Theoretical explanation of I-mode impurity removal</td>
<td></td>
<td>3</td>
<td>(^3)</td>
</tr>
<tr>
<td>II</td>
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<td>Pedestal poloidal variation captured neoclassically</td>
<td>2D (\parallel) dynamics</td>
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Appendix B

Parallel inertial term

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B.1 Parallel inertial term

In this appendix, it is verified that the inertial term contribution can be neglected when flux surface averaging the parallel momentum equation (3.8) multiplied by $\frac{B}{n_x}$ to obtain (3.7).

The inertial term is algebraically manipulated to achieve this aim, by using the followings vectorial relationships among generic vectors $a$ and $A$:

$$a \times (\nabla \times a) = \nabla \left( \frac{a^2}{2} \right) - a \cdot \nabla a \quad (B.1)$$

and

$$a \cdot \nabla \times A = \nabla \cdot (A \times a) + A \cdot \nabla \times a. \quad (B.2)$$

First, the inertial term can be rewritten by using (B.1) to find

$$V_z \cdot \nabla V_z \cdot B = B \cdot \nabla \left( \frac{V_z^2}{2} \right) - B \times V_z \cdot \nabla \times V_z.$$

Here the flux surface average of the first term vanishes and, by using (B.2), the second can be expressed as

$$B \times V_z \cdot (\nabla \times V_z) = \nabla \cdot (BV_z^2 - BV_z \parallel V_z) + V_z \cdot \nabla \times (B \times V_z). \quad (B.3)$$

When flux surface averaging the divergence of a vector, only its component in the direction perpendicular to the flux surface survives. Consequently, the flux surface average of the first term in (B.3) is negligible since the radial impurity flux is neglected (5.41). The second term can be also neglected since impurity diamagnetic effects are not allowed to compete with the $E \times B$ drift in the impurity flow (5.41), leading to

$$\nabla \times (B \times V_z) = -c \nabla \times \left( \frac{\partial \Phi}{\partial \psi} \nabla \psi \right).$$
This vanishes to lowest order, because the poloidal variation of the potential is small compared to the radial variation \cite{15, 23, 25, 27}, and the curl of the potential gradient is zero.

In conclusion, the inertial term contribution to the flux surface averaged parallel momentum conservation equation can be ignored because the radial impurity flux and the impurity diamagnetic effects are neglected \cite{5, 41}. 
Appendix C

Main ion kinetic equation and friction

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C.1 First-order main ion kinetic equation and friction force

The gyroaveraged background ion distribution function is given by \( \bar{f}_i = f_{iM(0)} + \bar{f}_{i1} \) [15, 24]. The lowest order distribution function can be chosen to be a stationary Maxwellian and a flux function:

\[
\bar{f}_{iM(0)} = \langle n_i \rangle (\psi) \left[ \frac{M_i}{2\pi T_i(\psi)} \right]^{\frac{3}{2}} \exp \left( -\frac{M_i v_i^2}{2T_i(\psi)} \right). \tag{C.1}
\]

The gyrophase independent first-order correction is proven [76] to be given by

\[
v_i \parallel \nabla \left( \bar{f}_{i1} + \frac{I_{v_i}}{\Omega_i} \frac{\partial f_{iM(0)}}{\partial \psi} \bigg|_{E_i(0)} \right) + \frac{z_i e v_i}{T_i} f_{iM(0)} \nabla \Phi = C_{i1} \{ \bar{f}_{i1} \} + C_{i21} \{ \bar{f}_{i1} \}. \tag{C.2}
\]

Here the spatial gradients are taken keeping constant the magnetic moment, \( \mu_i = \frac{v_i^2}{2B} \), and the lowest-order total energy, \( E_i(0) = \frac{v_i^2}{2} + \frac{z_i e \langle \Phi \rangle}{M_i} \). In addition, the linearized gyroaveraged unlike collision operator of bulk ions with lowest-order drifting Maxwellian impurities is

\[
C_{i21} \{ \bar{f}_{i1} \} = \frac{3\sqrt{2\pi \nu_{i1} T_i^3}}{4M_i^2} \left[ \nabla v_i \cdot (\nabla v_i \nabla v_i \cdot \nabla v_i \bar{f}_{i1}) + 2f_{iM(0)} \frac{M_i v_i \parallel v_i}{v_i^3} V_{z\parallel} \right]. \tag{C.3}
\]

The parallel friction force between impurities and the background ions is calculated [76] by taking the parallel first order moment of the unlike collision operator (C.3) to be given by

\[
R_{z\parallel} = -\langle p_i \rangle \frac{I_{v_{i1}}}{\Omega_i} \left[ \frac{d \ln \langle p_i \rangle}{d\psi} + \frac{z_i e d \langle \Phi \rangle}{T_i d\psi} - \frac{3}{2} \frac{d \ln T_i}{d\psi} \right] + M_i \nu_{i1} \langle n_i \rangle \left( \frac{n_i}{\langle n_i \rangle} u_B - V_{z\parallel} \right), \tag{C.4}
\]

where for general collisionality main ions

\[
u = \frac{3\sqrt{\pi}}{\sqrt{2}} \frac{T_i^3}{M_i^2} \int \frac{h_i v_i \parallel d^3 v_i}{B v_i^3} \tag{C.5}
\]
APPENDIX C. MAIN ION KINETIC EQUATION AND FRICTION

with

\[ h_i = \tilde{f}_i + \frac{I_{v_{\parallel}}}{\Omega_i} \frac{\partial f_{iM(\langle \rangle)}}{\partial \psi} \bigg|_{E_{i(\langle \rangle)}} + \frac{z_i e (\Phi - \langle \Phi \rangle)}{T_i} f_{iM(\langle \rangle)}. \]  

(C.6)

In particular, for banana bulk ions \( h_i \) does not depend on poloidal angle but via \( v_{\parallel} / |v_{\parallel}| \). Consequently, \( u \) is a flux function since \( d^3v_i \propto \frac{B}{v_{\parallel}^2} d\mu_i dE_{i(\langle \rangle)} \) [15].
Appendix D

Maxwellian impurity distribution function

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D.1 Maxwellian impurity distribution function to lowest order

In order for the impurity distribution function to be a drifting Maxwellian to lowest order, 

\[ f_{zM} = n_z \left( \frac{M_z}{2\pi T_z} \right)^{\frac{3}{2}} \exp \left( -\frac{M_z w_z^2}{2T_z} \right), \]  

(D.1)

its first-order correction \( f_{z1} \) should be much smaller. In this appendix, the implied parameter requirements are deduced from the static Fokker-Planck equation in spatial and relative velocity, \( w_z = v_z - V_z \), variables [78]:

\[
\begin{align*}
  v_z \cdot \nabla f_z + \left[ \Omega_z w_z \times \frac{B}{B} + \frac{z_e c}{M_z} \left( \frac{V_z \times B}{c} - v_z \cdot \nabla V_z \right) \right] \cdot \nabla_{w_z} f_z = & C_{zz} + C_{zi}; \\
  \nabla_{w_z} = & \frac{B}{B} \frac{\partial}{\partial w_{z||}} + \frac{w_{z\perp}}{w_{z\perp}} \frac{\partial}{\partial w_{z\perp}} - \frac{1}{w_{z\perp}} w_z \times \frac{B}{B} \frac{\partial}{\partial \varphi_z} 
\end{align*}
\]

(D.2)

with the gyrophase \( \varphi_z \) defined by \( w_{z\perp} = \nabla_{iz} \mathcal{E} \cos \varphi_z + \frac{B_z \nabla \psi}{B_{iz}} \sin \varphi_z \). It is convenient to decompose the first-order distribution function into its gyroaverage, \( \tilde{f}_{z1} = \langle f_{z1} \rangle_{\varphi_z} = \frac{1}{2\pi} \int d\varphi_z f_{z1} \), and gyrophase dependent part, \( f_{z1} = f_{z1} - \tilde{f}_{z1} \).

D.1.1 Gyrophase independent first-order correction:

The gyroaveraged first-order kinetic equation for the impurities is thus

\[
\begin{align*}
  w_{z||} \cdot \nabla f_{zM} - \frac{z_e c}{M_z B} \nabla \Phi \frac{\partial f_{zM}}{\partial w_{z||}} = & C_{zz1} \left\{ \tilde{f}_{z1} \right\} + \left\langle C_{zi1} \left\{ f_{i1} \right\} \right\rangle_{\varphi_z}; \\
  \nabla_{w_z} \sim & \frac{B}{B} \frac{\partial}{\partial w_{z||}} + \frac{w_{z\perp}}{w_{z\perp}} \frac{\partial}{\partial w_{z\perp}} - \frac{1}{w_{z\perp}} w_z \times \frac{B}{B} \frac{\partial}{\partial \varphi_z} 
\end{align*}
\]

(D.3)

since the other left hand side terms are negligible:

\[
\begin{align*}
  \frac{V_z \cdot \nabla f_{zM}}{w_{z||}} \sim & \frac{\frac{w_{z||}}{2} \frac{\partial f_{zM}}{\partial w_{z||}}}{w_{z||}} \cdot V_z \\
  \frac{w_{z||} \cdot \nabla f_{zM}}{w_{z||} \cdot \nabla f_{zM}} & \sim \frac{\frac{w_{z\perp}}{2} \frac{\partial f_{zM}}{\partial w_{z\perp}} - w_{z||} \frac{\partial f_{zM}}{\partial w_{z||}}}{w_{z\perp} \cdot \nabla f_{zM}} \\
  & \sim \frac{\rho_{yz}}{L_{nz}} \ll 1,
\end{align*}
\]

(D.5)
and
\[
\frac{-V_z \cdot \nabla V_z \cdot \frac{B}{B} \frac{\partial f_{zM}}{\partial w_z \parallel}}{w_z \parallel \cdot \nabla f_{zM}} \sim \frac{\rho_{pz}^2}{L_{nz}^2} \ll 1. \tag{D.6}
\]

So as to perform the gyroaverage, it has been used that \( \langle w_{z \perp} w_{z \perp} \rangle = w_{z \perp}^2 \left( I - \frac{B}{B \parallel} \right) \) and that \( I : \nabla V_z = \nabla \cdot V_z \), where \( I \) is the identity matrix. In order to calculate the estimates, it is worth recalling that the impurity density presents the strongest poloidal and poloidal variation. In addition, the relative velocity is of the order of the impurity thermal velocity in all directions.

If the parallel streaming and radial electric field terms balance self-collisions in (D.4), the size of the gyrophase independent first-order correction to the lowest-order impurity distribution function is given by
\[
\frac{\tilde{f}_{z1}}{f_{zM}} \sim \Delta \frac{v_{Tz}}{v_{zz} qR} \sim \Delta \frac{\lambda_z}{qR} \ll 1; \tag{D.7}
\]
while if unlike collisions balance self-collisions then
\[
\frac{\tilde{f}_{z1}}{f_{zM}} \sim \frac{\nu_{zi}}{v_{zz}} \sim \sqrt{\frac{z_i}{z_z}} \ll 1, \tag{D.8}
\]
which justifies the highly charged impurity assumption.

### D.1.2 Gyrophase dependent first order correction:

Subtracting from the Fokker-Planck equation (D.2) its flux surface average, the gyrophase dependent first-order kinetic equation for the impurities is thus given by
\[
w_{z \perp} \cdot \nabla f_{zM} + \frac{\nabla p_{z}}{M_{z} n_{z}} \cdot \frac{w_{z \perp}}{w_{z \perp} \partial w_{z \perp}} - \Omega_z \frac{\partial f_{z1}}{\partial \varphi_z} = C_{z11} \{ f_{11} \} - \langle C_{z11} \{ f_{11} \} \rangle \varphi_z ; \tag{D.9}
\]
where the following terms have been neglected on the left hand side:
\[
-\frac{-w_{z \perp} \cdot \nabla V_z \cdot \frac{B}{B} \frac{\partial f_{zM}}{\partial w_z \parallel}}{w_z \parallel \cdot \nabla f_{zM}} \sim \frac{\rho_{pz}}{L_{nz}} \ll 1 \tag{D.10}
\]
APPENDIX D. MAXWELLIAN IMPURITY DISTRIBUTION FUNCTION

\[ \frac{1}{w_{z\perp}} \frac{\partial f_{zM}}{\partial w_{z\perp}} \left[ \frac{w_{z\perp}^2}{2} \left( I - \frac{B B}{B} \right) - w_{z\perp} w_{z\perp} \right] \cdot \nabla f_{zM} \sim \frac{\rho z}{L_{n_z}} \ll 1, \tag{D.11} \]

with \( a_1 a_2 : \nabla V_z = a_2 \cdot \nabla V_z \cdot a_1 \) for generic vectors \( a_1 \) and \( a_2 \). Moreover, the perpendicular momentum conservation is assumed in (5.15) to be dominated by the Lorentz, electrostatic and isotropic pressure forces:

\[ \frac{\nabla \cdot \pi_{zM} - R_{zi M_{i n}}}{\omega_{z \perp}} \frac{\partial f_{zM}}{\partial w_{z\perp}} \sim \frac{\nabla \cdot \pi_{zM}}{\omega_{z \perp}} \frac{\partial f_{zM}}{\partial w_{z\perp}} \ll 1. \tag{D.12} \]

Finally, the term containing the gyrofrequency overtakes the like collision operator since

\[ \frac{C_{z11} \{ \tilde{f}_{z1} \}}{\Omega_z \frac{\partial f_{z1}}{\partial \phi_z}} \sim \frac{\nu_{zz}}{\Omega_z} \ll 1. \tag{D.13} \]

If the term involving the gyrofrequency competes with the perpendicular streaming in (D.9), the size of the gyrophase dependent first-order correction to the impurity distribution function is given by

\[ \frac{\tilde{f}_{z1}}{f_{zM}} \sim \frac{\nu_T z}{\Omega_z L_{n_z}} \sim \frac{\rho z}{L_{n_z}} \ll 1, \tag{D.14} \]

while if the former balances unlike collisions then

\[ \frac{\tilde{f}_{z1}}{f_{zM}} \sim \frac{\nu_{zi} f_{zM} f_{z1} - \langle f_{z1} \rangle}{\Omega_z f_{z1} f_{iM}} \sim \frac{\nu_{zz} f_{z1} - \langle f_{z1} \rangle}{\Omega_z f_{iM}} \sim \frac{\rho z f_{z1} - \langle f_{z1} \rangle}{\lambda_z f_{iM}} \ll 1; \tag{D.15} \]

where it has been used that \( f_{zM} \sim \sqrt{\frac{\nu_{z1}}{\nu_{zi}}} \) for the orderings in hand. This is satisfied automatically since \( \rho z \ll \lambda_z \).
Appendix E

Heat flux and viscous contributions

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E.1 Neglecting heat flux and viscous contributions to the parallel momentum and energy conservation equations

In this appendix, it is justified that the divergence of the heat flux does not significantly affect the impurity energy balance (7.5) for the new orderings. Furthermore, the anisotropic force and the viscous dissipation are proven to be negligible contributions to the impurity parallel momentum (5.33, 5.34) and energy (7.3, 7.4) conservation respectively, by using the calculated impurity flux (5.41).

Although there may be additional components coming from the presence of unlike collisions on the impurity Fokker-Planck equation, the most complete expressions for the collisional heat flux and viscous tensor to date [78] are used for the estimates.

E.1.1 Heat flux

The collisional and diamagnetic heat flux obtained in Eq. 39 of [78] (C),

\[ \mathbf{q}_{\text{C}} = \frac{p_z}{M_z} \left( -\frac{125}{32\nu_{zz}} \frac{\mathbf{B} \cdot \nabla T_z}{B^2} + \frac{5}{2\Omega_z} \frac{\mathbf{B} \times \nabla T_z}{B} - \frac{2\nu_{zz}}{\Omega_z^2} \mathbf{\nabla}_\perp T_z \right), \]  

(E.1)

has the following size in the parallel, poloidal and radial directions:

\[ \mathbf{q}_{\text{C}} \parallel \sim -\frac{p_z T_z}{M_z \nu_{zz}} \frac{\mathbf{B} \cdot \nabla \theta \partial \ln T_z}{\partial \theta}, \]
\[ \mathbf{q}_{\text{C}} \cdot \mathbf{B} \times \nabla \psi \sim \frac{p_z R B_p}{M_z \Omega_z} \left( \frac{\partial T_z}{\partial \psi} + \frac{\nabla \theta \cdot \nabla \psi \partial T_z}{R^2 B_p^2 \partial \theta} \right), \]
\[ \mathbf{q}_{\text{C}} \cdot \nabla \psi \sim \frac{p_z T_z \mathbf{B} \times \nabla \theta \cdot \nabla \psi \partial \ln T_z}{M_z \Omega_z \mathbf{B} R B_p} \partial \theta, \]

\[ \sim p_z v_{T z} \frac{\lambda_z \partial \ln T_z}{q R} \partial \theta, \]
\[ \sim p_z v_{T z} \frac{z_i \rho_z}{T_{n z}}, \]
\[ \sim p_z v_{T z} \frac{z_i \rho_z}{q R} \partial \ln T_z. \]  

(E.2)
Due to axisymmetry, the size of the divergence of the heat flux is thus given by

\[
\nabla \cdot q_{zC} = B \cdot \nabla \theta \left[ \frac{\partial}{\partial \theta} \left( q_{zC} \cdot \nabla \theta \right) + \frac{\partial}{\partial \psi} \left( \frac{q_{zC}}{B} \cdot \nabla \psi \right) \right] \\
\sim \frac{p_z v_T}{qR} \max \left\{ \Delta \frac{\lambda_z}{z_{n_z}} \frac{\partial \ln T_z}{\partial \theta}, \Delta \frac{z_{i_z}}{z_{n_z}} \rho_{pz} \frac{\partial \ln T_z}{\partial \theta} \right\} , \quad (E.3)
\]

where (5.18) and the fact that the strongest radial and poloidal variation are exhibited by the impurity density have been used.

### E.1.2 Viscous tensor

**Diagonal:** The diagonal \((d)\) part of the viscous tensor is obtained on Eq. (42) of [78]:

\[
\pi_{zdC} \cdot \frac{B}{B} = \frac{2B}{3B} \left\{ \frac{M_z}{p_z T_z} \left( 0.412 q_{z||C}^2 - 0.064 q_{zC}^2 \right) \right. \\
\left. + \frac{0.960}{\nu_{zz}} \left( I - 3 \frac{BB}{BB} \right) \left[ 0.246 \left( \nabla q_{zC} - q_{zC} \nabla \ln p_z + \frac{4}{15} \nabla q_{z||C} \right) \right] \right. \\
\left. + \left( p_z \nabla V_z + \frac{2}{5} \nabla q_{zC} \right) \right\} .
\]

(E.4)

It contains heat flux (E.3) and impurity flux (7.8) terms, whose size ratios are given by

\[
\frac{M_z}{p_z T_z} q_{zC}^2 \sim \frac{1}{\Delta} \max \left\{ \frac{\lambda_z}{qR} \frac{L_{n_z}}{\rho_{pz}} \left( \frac{\partial \ln T_z}{\partial \theta} \right)^2, \frac{qR}{\lambda_z} \frac{L_{n_z}}{\nu_{zz}} \frac{z_{i_z}}{z_{n_z}} \frac{B_p^2}{B^2}, \frac{\lambda_z}{qR} \frac{\partial \ln T_z}{\partial \theta} \right\} 
\]

(E.5)

and

\[
\frac{1}{\nu_{zz}} \nabla \cdot q_{zC} \sim \max \left\{ \frac{\lambda_z}{qR} \frac{L_{n_z}}{\rho_{pz}} \frac{\partial \ln T_z}{\partial \theta}, \frac{z_i}{z_{n_z}} \frac{\partial \ln T_z}{\partial \theta} \right\} .
\]

(E.6)

The size of the viscous tensor diagonal term, for Maxwell-Boltzmann main ions (5.13), is thus given by

\[
\frac{B_B}{B_B} \cdot \pi_{zdC} \cdot \frac{B_B}{B_B} \sim \max \left\{ 1, \frac{\lambda_z}{qR} \frac{L_{n_z}}{\rho_{pz}} \frac{\partial \ln T_z}{\partial \theta}, \frac{1}{\Delta \lambda_z} \frac{L_{n_z}}{qR} \left( \frac{\partial \ln T_z}{\partial \theta} \right)^2 \right\} ,
\]

(E.7)

where the size of the divergence of the impurity flux is calculated on (7.8).
APPENDIX E. HEAT FLUX AND VISCOS CONTRIBUTIONS

The contribution of the diagonal viscous tensor to the viscous force is thus indeed negligible compared to the pressure and potential gradients in the parallel momentum equation,

\[
\nabla \cdot \pi_{zdC} \cdot \frac{B}{B} \nabla z \sim \max \left\{ \frac{\rho_{pz}}{L_{n_z}} \frac{\lambda_z}{qR} \left( \frac{\Delta \lambda_z}{qR} \right)^2 1 \frac{\partial \ln T_z}{\partial \theta}, \left( \frac{\rho_{pz} \partial \ln T_z}{qR} \partial \theta \right)^2 \right\} \ll 1, \quad (E.8)
\]

since the strongest poloidal variation of the viscous tensor is dictated by the impurity density. Additionally, the correspondent viscous energy is also actually negligible with respect to the compressional heating in the energy equation,

\[
\pi_{zdC} : \nabla V_z = \frac{3}{2} \left( \frac{B}{B} \nabla V_z \cdot \frac{B}{B} - \frac{\nabla \cdot V_z}{3} \right) \frac{B}{B} \cdot \pi_{zdC} \cdot \frac{B}{B}. \quad (E.10)
\]

**Off-diagonal:** On the one hand, the off-diagonal or gyroviscous \((g)\) part of the viscous tensor is obtained on Eq. (44) of [78]:

\[
\pi_{zdC} = \frac{p_z}{4\Omega_z} \left\{ \frac{B}{B} \nabla V_z + \frac{2}{5} \frac{\nabla q_{zc}}{p_z} \right\} \left( I + 3 \frac{B}{B} \frac{B}{B} \nabla V_z \cdot \frac{B}{B} \right) - \left( I + 3 \frac{B}{B} \frac{B}{B} \right) \left[ \left( \nabla V_z + \frac{2}{5} \frac{\nabla q_{zc}}{p_z} \right) \left( \nabla V_z + \frac{2}{5} \frac{\nabla q_{zc}}{p_z} \right)^T \right] \times \frac{B}{B}. \quad (E.11)
\]

In order to identify the dominant terms, it is worth bear in mind that the ratio impurity heat flux divided by the pressure to mean flow \((5.29, 5.20, 5.19)\) has the following size in each direction \((5.18)\):

\[
\frac{\nabla \cdot \nabla V_z}{\nabla \cdot V_z} \sim \frac{125 p_z}{32 M_{\nu_z} B} \frac{B}{B} \nabla T_z \sim \frac{\lambda_z}{qR} \frac{\partial \ln T_z}{\partial \theta} \frac{L_{n_z}}{p_{pz}}, \quad (E.12)
\]

\[
\frac{\nabla \cdot \nabla V_z}{\nabla \cdot V_z} \sim \frac{5 p_z}{2 M_{\nu_z} B} \times \frac{B}{B} \cdot \nabla T_z \cdot \frac{B}{B} \frac{\nabla \psi}{BR^p} \sim \frac{z_i}{z_z} \ll 1 \quad (E.12)
\]

\[
\frac{\nabla \cdot \nabla V_z}{\nabla \cdot V_z} \sim \frac{5 p_z}{2 M_{\nu_z} B} \times \frac{B}{B} \cdot \nabla T_z \cdot \frac{\nabla \psi}{BR^p} \sim \frac{\partial \ln T_z}{\partial \theta} \Delta \ll 1.
\]
The size of the gyroviscous force in the parallel momentum equation is represented by the following term:

\[
\nabla \cdot \pi_{zgC} \cdot \frac{B}{B} \sim \nabla p_z \cdot \frac{B}{B} \times \left[ \left( \nabla V_z + \frac{2}{5} \frac{\nabla q_z C}{p_z} \right) + \left( \nabla V_z + \frac{2}{5} \frac{\nabla q_z C}{p_z} \right)^T \right] \cdot \frac{B}{B}, \tag{E.13}
\]

where the term with the magnetic field brought inside the gradient is used since the impurity density presents the strongest radial and poloidal variation. More specifically, the untransposed term in (E.13),

\[
\nabla p_z \cdot \frac{B}{B} \times \left( \nabla V_z + \frac{2}{5} \frac{\nabla q_z C}{p_z} \right) \sim \frac{\Delta p_z}{qR} \frac{\rho_{pz}}{L_{nz}} \max \left\{ \frac{\rho_{pz}}{L_{nz}}, \frac{\lambda_z}{qR} \frac{\partial \ln T_z}{\partial \theta} \right\}, \tag{E.14}
\]

dominates the transposed one,

\[
\left( \nabla \frac{\|V_z}{\|} + \frac{2}{5} \frac{\nabla q_z C}{p_z} \right) \times \frac{B}{B} \cdot \frac{\nabla p_z}{\Omega_z} \sim \frac{\Delta p_z}{qR} \frac{\rho_{pz}^2}{L_{nz}^2}, \tag{E.15}
\]

whose size has been estimated by using (E.12) and noticing that

\[
\nabla \cdot \nabla \psi \cdot \frac{B^2}{B} \cdot \nabla \ln n_z \sim \frac{\Delta p_z}{qR} \frac{\rho_{pz}}{L_{nz}} v_T R^z B^2 \frac{\partial \ln n_z}{\partial v} \sim \left( \frac{\Delta L_{nz}}{eR} \right)^2 \ll 1. \tag{E.16}
\]

In conclusion, the gyroviscous force can indeed be successfully neglected in the parallel momentum equation:

\[
\nabla \cdot \pi_{zgC} \cdot \frac{B}{B} \nabla \nabla \parallel p_z + z_v \nabla n_z \nabla \Phi \sim \max \left\{ \frac{\rho_{pz}^2}{L_{nz}^2}, \frac{\rho_{pz}}{L_{nz}^2} \frac{\lambda_z}{qR} \frac{\partial \ln T_z}{\partial \theta} \right\} \ll 1. \tag{E.17}
\]

The size of the gyroviscous energy can be estimated by using the following terms since the strongest variation of the impurity flow is given by the impurity density:

\[
\pi_{zgC} \cdot \nabla V_z \sim V_z \cdot \frac{B}{B} \times \left[ \left( \nabla V_z + \frac{2}{5} \frac{\nabla q_z C}{p_z} \right) + \left( \nabla V_z + \frac{2}{5} \frac{\nabla q_z C}{p_z} \right)^T \right] \cdot \frac{\nabla p_z}{4 \Omega_z}
- V_z \left[ \nabla V_z + \left( \nabla V_z + \frac{2}{5} \frac{\nabla q_z C}{p_z} \right)^T \right] \times \frac{B}{B} \cdot \frac{\nabla p_z}{4 \Omega_z}. \tag{E.18}
\]
Here it has been used that the perpendicular mean flow is larger than the perpendicular heat flux (E.12). The size of each term in (E.18) is calculated by using also (7.8) and (E.16):

\[
\mathbf{V}_z \cdot \mathbf{B} \times \left( \nabla \mathbf{V}_z + \frac{2}{5} \frac{\nabla q_{le}}{p_z} \right) \cdot \frac{\nabla p_z}{4\Omega_z} = \frac{\Delta p_z v_T z}{q R} \frac{\rho_z}{L_{n_z}} \frac{\lambda_z}{q R} \frac{\partial \ln T_z}{\partial \theta} \max \left\{ \frac{\rho_p z}{L_{n_z}}, \frac{\lambda_z}{q R} \frac{\partial \ln T_z}{\partial \theta} \right\}.
\]

\[
\nabla p_z \cdot \nabla V_{z \perp} \times \frac{\mathbf{B}}{B} \cdot \mathbf{V}_{z \perp} \sim \frac{\Delta p_z v_T z}{q R} \frac{\rho_z}{L_{n_z}} \frac{\lambda_z}{q R} \frac{\partial \ln T_z}{\partial \theta} \max \left\{ \frac{\rho_p z}{L_{n_z}}, \frac{\lambda_z}{q R} \frac{\partial \ln T_z}{\partial \theta} \right\}.
\]

\[
\nabla p_z \cdot \nabla V_z \times \frac{\mathbf{B}}{B} \cdot \mathbf{V}_z \sim \frac{\Delta p_z v_T z}{q R} \frac{\rho_z}{L_{n_z}} \frac{\lambda_z}{q R} \frac{\partial \ln T_z}{\partial \theta} \max \left\{ \frac{\rho_p z}{L_{n_z}}, \frac{\lambda_z}{q R} \frac{\partial \ln T_z}{\partial \theta} \right\}.
\]

(E.19)

The viscous energy can hence be neglected in the energy conservation equation since

\[
\frac{\pi_{zg C}}{p_z \nabla \cdot \mathbf{V}_z} \sim \max \left\{ \frac{\rho_p z}{L_{n_z}}, \frac{\lambda_z}{q R} \frac{\partial \ln T_z}{\partial \theta} \right\} \ll 1.
\]
Appendix F

Derivation of the impurity flow

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  F.1.4 Parallel impurity flow calculation . . . . . . . . . . . . . 179
F.1 Checking assumptions of the derivation of the velocity

The perpendicular impurity flow,

$$V_{z\perp} = \frac{c}{B^2} B \times \left( \nabla \Phi + \frac{\nabla p_z + M_z n_z V_z \cdot \nabla V_z + \nabla \cdot \tau_z + R_{iz}}{z en_z} \right), \quad (F.1)$$

is simplified into (5.15) by assuming that the perpendicular projection of the inertia, friction and viscous force are negligible. The sizes of these terms are estimated a posteriori in this appendix by using the resulting impurity flow (5.41) to check the applicability of the approximations.

F.1.1 Neglected inertial term

The inertial term can be conveniently rewritten as a divergence, by using conservation of impurity particles (5.22), to find

$$n_z V_z \cdot \nabla V_z = \nabla \cdot \left( n_z V_z V_z \right). \quad (F.2)$$

The projection of the inertial contribution to the perpendicular impurity flow (F.1) in the directions perpendicular to the flux surface and within the latter but perpendicular to the magnetic field are then respectively given by:

$$\frac{B}{B} \times \frac{\nabla \cdot \left( n_z V_z V_z \right)}{\Omega z n_z} \cdot \frac{\nabla \psi}{RB_p} = -\frac{\nabla \cdot \left( n_z V_z V_z \cdot \frac{B \times \nabla \psi}{RB_p} \right)}{\Omega z n_z} + \frac{V_z}{\Omega z} \cdot \nabla \left( \frac{B \times \nabla \psi}{RB_p} \right) \cdot V_z \quad (F.3)$$

and

$$\frac{B}{B} \times \frac{\nabla \cdot \left( n_z V_z V_z \right)}{\Omega z n_z} \cdot \frac{B \times \nabla \psi}{BRB_p} = \nabla \cdot \left( \frac{n_z V_z V_z \cdot \frac{\nabla \psi}{RB_p}}{\Omega z n_z} \right) - \frac{1}{\Omega z z} V_z \cdot \nabla \left( \frac{\nabla \psi}{RB_p} \right) \cdot V_z. \quad (F.4)$$

Since the impurity density presents the strongest poloidal (5.5) and radial (5.9) variation, the first terms on the right hand of (F.3) and (F.4) are used to
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determine the size of the correspondent projection of the inertial contribution to the perpendicular impurity flow (5.23, 5.19, 5.20):

\[
\nabla \cdot \left( \frac{n_z V_z V_z \cdot B_x \nabla \psi}{\Omega z n_z} \right) \approx \frac{B \cdot \nabla \theta}{\Omega z n_z} \partial \psi \left( \frac{n_z V_z \cdot \nabla \psi V_z \cdot B_x \nabla \psi}{B \cdot \nabla \theta} \right) \sim \Delta \rho_{pz} qR \frac{\rho_z^2}{L_{nz}^2}
\]

and

\[
\nabla \cdot \left( \frac{n_z V_z V_z \cdot B_x \nabla \psi}{\Omega z n_z} \right) \approx \frac{B \cdot \nabla \theta}{\Omega z n_z} \partial \theta \left( \frac{n_z V_z \cdot \nabla \theta V_z \cdot B_x \nabla \psi}{B \cdot \nabla \theta} \right) \sim \Delta \rho_{pz} qR \frac{\rho_z^2}{L_{nz}^2}.
\]

In conclusion, the projection of the inertial contribution to the perpendicular impurity flow (F.1) can be successfully neglected since

\[
\nabla \cdot \left( \frac{n_z V_z V_z \cdot B_x \nabla \psi}{\Omega z n_z} \right) \approx \frac{B \cdot \nabla \theta}{\Omega z n_z} \partial \psi \left( \frac{n_z V_z \cdot \nabla \psi V_z \cdot B_x \nabla \psi}{B \cdot \nabla \theta} \right) \sim \Delta \rho_{pz} qR \frac{\rho_z^2}{L_{nz}^2} \ll 1 \quad (F.7)
\]

and

\[
\nabla \cdot \left( \frac{n_z V_z V_z \cdot B_x \nabla \psi}{\Omega z n_z} \right) \approx \frac{B \cdot \nabla \theta}{\Omega z n_z} \partial \theta \left( \frac{n_z V_z \cdot \nabla \theta V_z \cdot B_x \nabla \psi}{B \cdot \nabla \theta} \right) \sim \Delta \rho_{pz} qR \frac{\rho_z^2}{L_{nz}^2} \ll 1. \quad (F.8)
\]

Inertial terms have zero flux surface average regardless of ordering.

F.1.2 Neglected friction term

The size of the components of the perpendicular friction in the direction perpendicular to the flux surface and perpendicular to the magnetic field but contained within the flux function are respectfully given by

\[
\nabla \cdot \left( \frac{n_z V_z V_z \cdot \nabla \psi}{\Omega z n_z} \right) \approx \frac{B \cdot \nabla \theta}{\Omega z n_z} \partial \psi \left( \frac{n_z V_z \cdot \nabla \psi V_z \cdot \nabla \psi}{B \cdot \nabla \theta} \right) \sim \Delta \rho_{pz} qR \frac{\rho_z^2}{L_{nz}^2} \ll 1 \quad (F.9)
\]
and
\[
\mathbf{R}_{iz} \cdot \frac{\mathbf{B} \times \nabla \psi}{BRB_p} = M_i \int d^3 v_i w_i \cdot \frac{\mathbf{B} \times \nabla \psi}{BRB_p} \left( C_{iz1} - \langle C_{iz1} \rangle \right) \sim M_i n_i \nu_{iz} v_T z \frac{\rho_p}{L_{nz}};
\]
\[(F.10)\]
since the gyrophase-dependent piece of the unlike collision operator (C.3) is
\[
C_{iz1} - \langle C_{iz1} \rangle = 3 \sqrt{\frac{2 \pi \nu_{iz} T_i}{4 M_i^2}} \left[ \nabla v_i \cdot \left( \nabla v_i \nabla v_i \cdot \nabla v_i \hat{f}_{i1} \right) + 2 f_{iM} \frac{M_i}{T_i} \frac{v_i \cdot v_i}{T_i} \right],
\]
\[(F.11)\]
with \( \hat{f}_{i1} = f_{i1} - \bar{f}_{i1} \) and the size of the perpendicular impurity flow dictated by (5.19) and (5.20). In conclusion, the contribution of the friction force to the perpendicular impurity flow (F.1) can be successfully neglected if
\[
\mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \sim 1\Delta B qR B \ll 1, \quad (F.12)
\]
which implies that (7.7)
\[
\mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \cdot \mathbf{B} \sim 1\Delta B qR B \ll 1. \quad (F.13)
\]
\[\text{F.1.3 Neglected viscous term}\]
\[\text{Diagonal terms:}\] The divergence of the viscous tensor dotted into the perpendicular directional vector can be related (5.18) to that of the parallel diagonal component, whose size is estimated on (E.7), to find
\[
\nabla \cdot \left( \pi_{zdC} \cdot \frac{\nabla \psi}{BRB_p} \right) = -\frac{1}{2} \nabla \cdot \left( \frac{\nabla \psi}{BRB_p} \cdot \pi_{zdC} \cdot \mathbf{B} \right) \sim \frac{1}{L_{nz}} \frac{B}{B} \cdot \pi_{zdC} \cdot \mathbf{B} \quad (F.14)
\]
and
\[
\nabla \cdot \left( \pi_{zdC} \cdot \frac{\mathbf{B} \times \nabla \psi}{BRB_p} \right) = -\frac{1}{2} \nabla \cdot \left( \frac{\mathbf{B} \times \nabla \psi}{BRB_p} \cdot \pi_{zdC} \cdot \mathbf{B} \right) \sim \frac{\Delta B}{qRB_p} \frac{B}{B} \cdot \pi_{zdC} \cdot \mathbf{B}. \quad (F.15)
\]
Consequently, the contribution of the diagonal terms of the viscous tensor to the perpendicular impurity flow (F.1) can be automatically neglected with no further
assumptions since
\[
\frac{\mathbf{B} \times \nabla \pi_{\text{AC}}}{M_{\Omega_{\text{AC}}}} \cdot \frac{\nabla \psi}{RB_p} = \frac{\mathbf{B} \times \nabla \pi_{\text{AC}}}{M_{\Omega_{\text{AC}}}} \cdot \frac{\nabla \psi}{RB_p} \sim \frac{\mathbf{B} \times \nabla \pi_{\text{AC}}}{M_{\Omega_{\text{AC}}}} \cdot \frac{\nabla \psi}{RB_p} = \frac{\mathbf{B} \times \nabla \psi}{M_{\Omega_{\text{AC}}}} \cdot \frac{\nabla \psi}{RB_p} \sim \\
\sim \max \left\{ \Delta \frac{\rho_{pz}}{L_n} \frac{\lambda_z}{qR}, \Delta \left( \frac{\lambda_z}{qR} \right)^2 \frac{\partial \ln T_z}{\partial \theta}, \left( \frac{\rho_{pz}}{qR} \frac{\partial \ln T_z}{\partial \theta} \right)^2 \right\} \ll 1. \quad (F.16)
\]

**Off-diagonal terms:** The size of the divergence of the dominant terms \([E.12]\) of the gyroviscous tensor dotted into the unitary vector perpendicular to the flux surface,
\[
\pi_{zgC} \cdot \frac{\nabla \psi}{RB_p} = \frac{p_z}{4\Omega_z} \left\{ \frac{\mathbf{B}}{B} \times \left[ \nabla V_z + \left( \nabla V_z \right)^T \right] \cdot \frac{\nabla \psi}{RB_p} \right\} - \left( I + 3 \frac{\mathbf{B} \cdot \mathbf{B}}{BB} \right) \cdot \left[ \nabla V_z + \left( \nabla V_z + \frac{2}{5} \nabla \frac{q_{zC}}{p_z} \right)^T \right] \cdot \frac{\mathbf{B} \times \nabla \psi}{RB_p} \right\}, \quad (F.17)
\]
is estimated by applying the gradient to the impurity pressure and analysing each term separately:
\[
\frac{\nabla p_z}{4\Omega_z} \cdot \frac{\mathbf{B}}{B} \times \nabla V_z \cdot \frac{\nabla \psi}{RB_p} \sim \frac{\Delta^2 p_z}{qR} \frac{\rho_{pz}}{qR} \frac{\rho_{pz}}{L_n^2}, \quad \frac{\nabla \psi}{RB_p} \cdot \nabla V_z \times \frac{\mathbf{B}}{B} \cdot \frac{\nabla p_z}{4\Omega_z} \sim \frac{p_z}{L_n} \frac{\rho_{pz}}{L_n^2}, \quad \frac{\nabla p_z}{4\Omega_z} \cdot \frac{\mathbf{B}}{B} \times \frac{\nabla \psi}{RB_p} \sim \frac{p_z}{L_n} \frac{\rho_{pz}}{L_n^2}.
\]

\[
\frac{\mathbf{B} \times \nabla \psi}{RB_p} \cdot \left( \nabla V_z + \frac{2}{5} \nabla \frac{q_{zC}}{p_z} \right) \cdot \frac{\nabla p_z}{4\Omega_z} \sim \frac{\Delta^2 p_z}{qR} \frac{\rho_{pz}}{qR} \frac{\rho_{pz}}{L_n} \max \left\{ \frac{\rho_{pz}}{L_n}, \frac{\lambda_z}{qR} \frac{\partial \ln T_z}{\partial \theta} \right\}. \quad (F.18)
\]

Analogously, the size of the divergence of the dominant terms \([E.12]\) of the gyroviscous tensor dotted into the unitary vector within the flux surface but perpendicular to the magnetic field,
\[
\pi_{zgC} \cdot \frac{\mathbf{B} \times \nabla \psi}{RB_p} = \frac{p_z}{4\Omega_z} \left\{ \frac{\mathbf{B}}{B} \times \left[ \nabla V_z + \left( \nabla V_z \right)^T \right] \cdot \frac{\mathbf{B} \times \nabla \psi}{RB_p} \right\} + \left( I + 3 \frac{\mathbf{B} \cdot \mathbf{B}}{BB} \right) \cdot \left[ \nabla V_z + \left( \nabla V_z + \frac{2}{5} \nabla \frac{q_{zC}}{p_z} \right)^T \right] \cdot \frac{\mathbf{B} \times \nabla \psi}{RB_p} \right\}, \quad (F.19)
\]
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is estimated term by term as follows:

\[
\begin{align*}
\nabla p_z \frac{B}{4 \Omega_z} \cdot \nabla \psi \cdot \frac{B \times \nabla \psi}{BRB_p} & \sim \frac{\Delta p_z}{qR} \frac{\rho_p z}{L_n z} \frac{\rho_z}{L_n z}, \\
\nabla p_z \frac{B}{4 \Omega z} \times \nabla \psi \cdot \frac{B \times \nabla \psi}{BRB_p} & \sim \frac{\Delta p_z}{qR} \frac{\rho_p z}{L_n z} \frac{\rho_z}{L_n z}, \\
\n\nabla p_z \frac{B}{4 \Omega z} \cdot \nabla \psi \cdot \frac{B \times \nabla \psi}{BRB_p} & \sim \frac{\Delta p_z}{qR} \frac{\rho_p z}{L_n z} \frac{\rho_z}{L_n z},
\end{align*}
\]

\[
\begin{align*}
\nabla \psi \cdot \left( p_z \nabla V_z + \frac{2}{5} \nabla q_z C \right) \cdot \nabla \ln n_z \frac{L_n z}{4 \Omega z} & \sim \frac{\Delta p_z}{qR} \frac{\rho_p z}{L_n z} \max \left\{ \frac{\rho_p z}{L_n z}, \frac{\lambda_z \partial \ln T_z}{qR} \right\}.
\end{align*}
\]

(F.20)

The contribution of the gyroviscous tensor to the perpendicular impurity flow (F.1) can hence be neglected as well since

\[
\begin{align*}
\frac{B}{B} \times \frac{\nabla p_z \pi_{\psi C}}{M_z \Omega_z n_z} \cdot \frac{\nabla \psi}{RB_p} & \sim \frac{\nabla p_z \pi_{\psi C}}{M_z \Omega_z n_z} \cdot \frac{\nabla \psi}{RB_p} \sim \frac{B_p}{B} \frac{\rho_p z}{L_n z} \max \left\{ \frac{\rho_p z}{L_n z}, \frac{\lambda_z \partial \ln T_z}{qR} \right\} \ll 1
\end{align*}
\]

(F.21)

and

\[
\begin{align*}
\frac{B}{B} \times \frac{\nabla p_z \pi_{\psi C}}{M_z \Omega_z n_z} \cdot \frac{\nabla \psi}{RB_p} & \sim \frac{\nabla p_z \pi_{\psi C}}{M_z \Omega_z n_z} \cdot \frac{\nabla \psi}{RB_p} \sim \max \left\{ \frac{\rho^2_p}{L^2_n z}, \frac{\Delta^2 p_z}{qR qR} \frac{\rho_p z}{qR qR} \frac{\lambda_z \partial \ln T_z}{\partial \theta} \right\} \ll 1.
\end{align*}
\]

(F.22)

F.1.4 Parallel impurity flow calculation

If the perpendicular projection of the inertia, friction and divergence of the anisotropic pressure tensor are negligible on the perpendicular momentum conservation (5.15), their correspondent contribution to the conservation of particles (5.23) are also negligible under the established orderings.
Appendix G

Collision operator

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G.1 Collision operator

In this appendix, attention is drawn to like and unlike collision operators between impurities and/or bulk ions. General distribution functions for those species are allowed, even though the insightful case in which they are a drifting Maxwellian to lowest order is also considered. Even though the impurity distribution function is a drifting Maxwellian to lowest order, a stationary Maxwellian is utilized to analyze the bulk ion behaviour. Thus, the following results could be trivially particularized for the situation in hand by setting the bulk ion mean flow to zero.

The primary focus of this analysis is an accurate calculation of the size of the different components of the linearized collision operators. The purpose is to determine the most important physics to be retained in kinetic or fluid equations. Second, properties such as rotationally symmetry are looked for in each component in order to facilitate a proper estimate of gyroaverages.

G.1.1 Impurity-impurity and main-main ion collision operator

The Landau form of the Fokker-Planck collision operator for like impurity collisions [76] is given by

\[
C_{zz}\{f_z\} = \frac{3\sqrt{\pi} \nu_{zz} T_z^2}{2n_z M_z^2} \nabla_{v_z} \cdot \left[ \int d^3 v'_z \nabla_g \nabla_g g \cdot \left( f'_z \nabla_{v_z} f_z - f_z \nabla_{v'_z} f'_z \right) \right]; \tag{G.1}
\]

where \( g = v_z - v'_z = w_z - w'_z \) and \( f'_z \) indicates that the distribution function is evaluated in \( v'_z \). Note that the lowest order linearized collision operator,

\[
C_{zz0}\{f_{z0}\} = \frac{3\sqrt{\pi} \nu_{zz} T_z^2}{2n_z M_z^2} \nabla_{v_z} \cdot \left[ \int d^3 v'_z \nabla_g \nabla_g g \cdot \left( f'_{z0} \nabla_{v_z} f_{z0} - f_{z0} \nabla_{v'_z} f'_{z0} \right) \right] \tag{G.2}
\]

\sim \nu_{zz} f_{z0},

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vanishes if the lowest order distribution function is a Maxwellian, since \( \nabla_v f_{zM} = -\frac{M_z}{T_z} w_z f_{zM} \) and
\[
\nabla_g \nabla_g g \cdot g = \frac{g^2 I - gg}{g^3} \cdot g = 0. \tag{G.3}
\]
The first order linearized collision operator,
\[
\frac{C_{zz1} \{ f_{z1} \}}{\sqrt{\pi} \nu_{zz} T_z^3} = \nabla_{v_z} \cdot \left\{ f_{z0} \int d^3v_z f'_{z0} \nabla_g \nabla_g \cdot \left[ \nabla_{v_z} \left( \frac{f_{z1}}{f_{z0}} \right) - \nabla_{v_z'} \left( \frac{f'_{z1}}{f'_{z0}} \right) \right] \right\}
\]
\[
\sim \nu_{zz} f_{z1}, \tag{G.4}
\]
is obtained by evaluating \( C_{zz} \left\{ f_{zM} \left( 1 + \frac{f_{z1}}{f_{zM}} \right) \right\} \) and neglecting \( O \left[ \frac{f_{z1}}{f_{zM} \nu_{zz} f_{z1}} \right] \) corrections afterwards. This linearized collision operator is rotationally symmetric, so the only way of introducing a preferred direction is through \( f_{z1} \). As a consequence, it verifies the following property:
\[
\langle C_{zz1} \{ f_{z1} \} \rangle_\varphi = C_{zz1} \left\{ \langle f_{z1} \rangle_\varphi \right\}. \tag{G.5}
\]
Finally, note that the results are analogous for like collisions between two background ions.

### G.1.2 Background ion-impurity collision operator

The Landau form of the Fokker-Planck collision operator of background ions with impurities \cite{footnote} is given by
\[
C_{iz} \{ f_i, f_z \} = \frac{3 \sqrt{2 \pi} \nu_{iz} T_i^3}{4 n_z M_i M_z^2} \nabla_{v_i} \cdot \left[ \int d^3v_z \nabla_g \nabla_g \cdot (M_z f_z \nabla_{v_z} f_i - M_i f_i \nabla_{v_z} f_z) \right]; \tag{G.6}
\]
where \( g = v_i - v_z = w_i + (V_i - V_z) - w_z \). The lowest order linearized collision operator,
\[
C_{iz0} \{ f_{i0}, f_{z0} \} = \frac{3 \sqrt{2 \pi} \nu_{iz} T_i^3}{4 n_z M_i^2} \nabla_{v_i} \cdot \left[ \int d^3v_z f_{z0} \nabla_{w_i} \nabla_{w_i} w_i \cdot \nabla_{v_i} f_{i0} \right] \sim \nu_{iz} f_{i0}, \tag{G.7}
\]
can be obtained by Taylor expanding $g$ over $w_i$ and neglecting small terms. Note that it cancels out if the lowest order distribution function for bulk ions is a Maxwellian (G.3).

If both impurity and bulk ion distribution functions are Maxwellian to lowest order, the collision operator can be simplified by using (G.3) to find

$$C_{iz} \{ f_{iM} + f_{i1}, f_{zM} \} = \frac{3\sqrt{2\pi} \nu_{iz} T_i^3}{4n_i M_i^2} \nabla_{v_i} \cdot \left\{ \int d^3v_z f_{zM} \nabla_g \nabla g \cdot \nabla_{v_i} f_{i1} \right\} +$$

$$+ \frac{3\sqrt{2\pi} \nu_{iz} T_i^{1.5}}{4n_i M_i^2} \nabla_{v_i} \cdot \left\{ f_{iM} \int d^3v_z f_{zM} \nabla_g \nabla g \cdot \left[ (\nabla_i - \nabla_z) + \left( \frac{T_i}{T_z} - 1 \right) w_z \right] \nabla_{v_i} f_{i1} \right\}. \quad (G.8)$$

It has been shown that the lowest order component of the linearized collision operator cancels out for a Maxwellian. The next order component can be obtained by Taylor expanding $g$ over $w_i$ and performing the integrals in impurity velocity space to obtain

$$C_{iz1} \{ f_{iM} + f_{i1}, f_{zM} \} = \frac{3\sqrt{2\pi} \nu_{iz} T_i^3}{4M_i^2} \nabla_{v_i} \cdot (\nabla_{w_i} \nabla_{w_i} w_i \cdot \nabla_{v_i} f_{i1})$$

$$+ \frac{3\sqrt{2\pi} \nu_{iz} T_i^{1.5}}{4M_i^2} \nabla_{v_i} \cdot (f_{iM} \nabla_{w_i} \nabla_{w_i} w_i) \cdot (\nabla_i - \nabla_z). \quad (G.9)$$

Here, it has been used that $\int d^3v_z f_{zM} w_z = 0$. This expression can be further simplified, by using (G.3) and $\nabla_{w_i} \cdot \nabla_{w_i} \nabla_{w_i} w_i = -2 \frac{w_i}{w_i}$, to find

$$C_{iz1} \{ f_{iM} + f_{i1}, f_{zM} \} = \frac{3\sqrt{2\pi} \nu_{iz} T_i^3}{4M_i^2} \nabla_{v_i} \cdot (\nabla_{w_i} \nabla_{w_i} w_i \cdot \nabla_{v_i} f_{i1}) \sim \nu_{iz} f_{i1}$$

$$+ \frac{2f_{iM} M_i w_i}{T_i} \frac{w_i}{w_i^3} \cdot (V_z - V_i) \sim \nu_{iz} f_{iM} \frac{|V_z - V_i|}{v_{Ti}}. \quad (G.10)$$

Here the size of each term is indicated on the right hand side. Note that even though the first component of this linearized collision operator is rotationally symmetric, i.e. the only way of introducing a preferred direction is through $f_{i1}$, the second component has a preferred direction introduced by the mean flow velocity.
G.1.3 Impurity - background ion collision operator

The Landau form of the Fokker-Planck collision operator of impurities with main ions \[76\] is given by

\[
C_{zi} \{ f_z, f_i \} = \frac{3 \sqrt{2 \pi \nu_{zi} T_i^3}}{8 n_i M_z M_i^3} \nabla_{v_z} \cdot \left[ \int d^3 v_i \nabla g \nabla g \cdot (M_i f_i \nabla_{v_z} f_z - M_z f_z \nabla_{v_i} f_i) \right],
\]

where \( g = v_z - v_i = w_z + (V_z - V_i) - w_i \). The lowest order linearized collision operator,

\[
C_{zi0} \{ f_{z0}, f_{i0} \} = -\frac{3 \sqrt{2 \pi \nu_{zi} T_i^3}}{8 n_i M_i^2} \nabla_{v_z} \cdot \left( f_{z0} \int d^3 v_i \nabla_{w_i} \nabla_{w_i} w_i \cdot \nabla_{w_i} f_{i0} \right) \sim \sqrt{\frac{z_i}{z_z}} \nu_{zi} f_{z0},
\]

can be obtained by Taylor expanding \( g \) over \(-w_i\) and neglecting small terms. Note that it cancels out if the main ion distribution function is a Maxwellian to lowest order \([G.3]\). In addition, it is worth pointing out that the impurity gyroaverage of this collision operator is not equal to the collision operator of the gyroaverage of the distribution function.

If both bulk ion and impurity distribution functions are Maxwellian to lowest order, the collision operator can be simplified by using \([G.3]\) as follows:

\[
C_{zi} \{ f_{zM}, f_{iM} + f_{i1} \} = -\frac{3 \sqrt{2 \pi \nu_{zi} T_i^3}}{8 n_i M_i^2} \nabla_{v_z} \cdot \left[ f_{zM} \int d^3 v_i \nabla g \nabla g \cdot \nabla_{v_i} f_{i1} \right] + \frac{3 \sqrt{2 \pi \nu_{zi} T_i^3}}{8 n_i M_i^2} \nabla_{v_z} \cdot \left[ f_{zM} \left( 1 - \frac{T_z}{T_i} \right) w_z + (V_z - V_i) \right] \cdot \int d^3 v_i f_{iM} \nabla g \nabla g \g .
\]

It has been shown that the lowest order component of the linearized collision operator cancels out for a Maxwellian. The next order component can be obtained by Taylor expanding \( g \) over \(-w_i\). This allows to separate the divergence in impurity...
velocity space and the integral in main ion velocity space to find

\[ C_{zi1} \{ f_{zM}, f_{iM} + f_{i1} \} = -\frac{3\sqrt{2}\pi\nu z_i T_i^2}{8n_i M_i^2} \nabla_{v_z} f_{zM} \cdot \int d^3 v_i \nabla_{w_i} \nabla_{w_i} w_i \cdot \nabla_{v_i} f_{i1} + \]

\[ + \frac{3\sqrt{2}\pi\nu z_i T_i^2}{8n_i M_i^2} \nabla_{v_z} \left\{ f_{zM} \left[ \left( 1 - \frac{T_i}{T_z} \right) w_z + (V_z - V_i) \right] \right\} : \int d^3 v_i f_{iM} \nabla_{w_i} \nabla_{w_i} w_i. \]

(G.14)

The integral in main ion velocity space can be performed, by noticing that the Maxwellian distribution function is isotropic, to obtain

\[ \int d^3 v_i f_{iM} \nabla_{w_i} \nabla_{w_i} w_i = \int d^3 v_i f_{iM} \frac{w_i^2 I - w_i w_i}{w_i^3} = \frac{2}{3} \int d^3 v_i f_{iM} \frac{w_i}{w_i} = \frac{4n_i M_i^2}{3\sqrt{2}\pi T_i^2} I. \]

(G.15)

As a consequence, the double product can be converted into a divergence by invoking that \( \nabla_{v_z} : I = \nabla_{v_z} \cdot q \) for a generic vector \( q \). Finally, the expression for the linearized impurity-bulk ion collision operator (G.14) can be further simplified by carrying out also the gradients in impurity velocity space to find

\[ C_{zi1} \{ f_{zM}, f_{i1} \} = \]

\[ = \frac{3\sqrt{2}\pi\nu z_i T_i^2}{4n_i M_i^2} f_{zM} \frac{M_z}{T_z} w_z \cdot \int d^3 v_i \nabla_{w_i} \nabla_{w_i} w_i \cdot \nabla_{v_i} f_{i1} \sim \nu z_i f_{zM} \sqrt{\frac{z_z f_{i1}}{z_i f_{iM}}} \]

\[ + \nu z_i \frac{1}{2} f_{zM} \frac{M_z}{T_z} w_z \cdot (V_i - V_z) \sim \nu z_i f_{zM} \frac{|V_i - V_z|}{v_{Tz}} \]

\[ + \nu z_i \frac{1}{2} f_{zM} \left( 1 - \frac{T_i}{T_z} \right) \left( 3 - \frac{M_z}{T_z} w_z^2 \right) \sim \nu z_i f_{zM}. \]

(G.16)

Here the size of each component is indicated on the right hand side. Note that this linearized collision operator is also rotationally asymmetric.

The lowest order linearized collision operator for unlike collisions of impurities
APPENDIX G. COLLISION OPERATOR

with the background is composed of a gyrophase independent part, \( f_{i1} \),

\[
\langle C_{zi1} \rangle \varphi = \frac{3\sqrt{2} \pi \nu z_i T_i^3}{8 n_i M_i^2} f_{zM} M_z T_z w_z \| B \| \cdot \int d^3 v_i \nabla w_i \cdot \nabla v_i f_{i1} \sim \nu z_i f_{zM} \sqrt{\frac{z_i}{z_i}} f_{iM} \\
+ \frac{\nu z_i}{2} f_{zM} M_z T_z \| w_z \| (V_{i\|} - V_{z\|}) \sim \nu z_i f_{zM} \frac{V_{i\|} - V_{z\|}}{v_{Tz}} \\
+ \frac{\nu z_i}{2} f_{zM} \left( 1 - \frac{T_i}{T_z} \right) \left( 3 - \frac{M_z}{T_z} w_{z*}^2 \right) \sim \nu z_i f_{zM},
\]

(G.17)

and a gyrophase dependent part,

\[
C_{zi1} - \langle C_{zi1} \rangle \varphi = \\
= \frac{3\sqrt{2} \pi \nu z_i T_i^3}{8 n_i M_i^2} f_{zM} M_z T_z w_{z\perp} \cdot \int d^3 v_i \nabla w_i \cdot \nabla v_i f_{i1} \sim \nu z_i f_{zM} \sqrt{\frac{z_i}{z_i}} f_{iM} \\
+ \frac{\nu z_i}{2} f_{zM} M_z T_z w_{z\perp} \cdot (V_i - V_z) \sim \nu z_i f_{zM} \frac{|V_i \perp - V_z \perp|}{v_{Tz}},
\]

(G.18)

Note that the gyroaverage has been taken in impurity velocity space.

Silvia Espinosa Gútiez (sesp@mit.edu) 186/214
Appendix H

In-out asymmetry boundaries in terms of physical parameters

Contents

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  H.1.1 First order equation ($\alpha = 2\epsilon$) . . . . . . . . . . . . . . . 188
  H.1.2 Second order equation ($\alpha \neq 2\epsilon$) . . . . . . . . . . . . . . . 190
H.1 Boundaries in terms of physical parameters

In this Appendix, the physical domain in $\alpha$, $g$ and $U$ space for which any or both of the solutions for the $D$ that corresponds to the impurity density becoming zero at some poloidal angle, given by (6.10) and (6.12), are non-negative are analytically derived.

H.1.1 First order equation ($\alpha = 2\epsilon$)

From (6.10), the impurity diamagnetic flow becomes zero, $D = 0$, at

$$U = -g \pm \sqrt{g^2 (2\epsilon)^2 - (1 + 2\epsilon)^2};$$  \hspace{1cm} (H.1)

which is only defined for $|g| \geq \frac{1+2\epsilon}{2\epsilon}$. The values of $D$ when approaching the asymptote that annihilates the denominator of (6.10) from the left and right are given as

$$\lim_{[U+g(1+2\epsilon)] \to 0^-} D = \lim_{[U+g(1+2\epsilon)] \to 0^-} \frac{-(1+2\epsilon)^2}{4\epsilon [g(1+2\epsilon) + U]} \to +\infty$$

and

$$\lim_{[U+g(1+2\epsilon)] \to 0^+} D = \lim_{[U+g(1+2\epsilon)] \to 0^+} \frac{-(1+2\epsilon)^2}{4\epsilon [g(1+2\epsilon) + U]} \to -\infty,$$

respectively. Moreover, the values of the dimensionless impurity diamagnetic flow for very large negative and positive values of $U$ are

$$\lim_{U \to -\infty} D \to +\infty$$

and

$$\lim_{U \to +\infty} D \to -\infty,$$

respectively. From this analysis, the regions in $g$ and $U$ space with physical $D$ are derived and sketched in Table H.1.
Table H.1: Roots of (6.10), applicable when $\alpha = 2\epsilon$, where the impurity density becomes zero at some poloidal angle with physical impurity diamagnetic flow as a function of $g$ and $U$. Each row corresponds to a region in $g$ domain. The schematics in the last column represent $D$ as a function of $U$. Here the thin horizontal line corresponds to the $D = 0$ axis. For the regions of $U$ where there is a physical solution, there is a thick line corresponding to a non-negative value of $D$. The absence of a thick line indicates that there is not any physical solution in this region of $U$. Maximum in-out impurity density asymmetries can be found at the boundaries of these unphysical regions.
H.1.2 Second order equation \((\alpha \neq 2\epsilon)\)

It follows from (6.12) that there are two different real solutions for \(D\) if

\[
(2\epsilon)^2 [g (1 + \alpha) + U]^2 + [(2\epsilon)^2 - \alpha^2] (1 + \alpha)^2 > 0.
\]

(H.2)

It is worth noticing that this inequality is always satisfied for \(\alpha < 2\epsilon\); while for \(\alpha > 2\epsilon\) there can be two imaginary solutions, two real solutions or a double real solution. Indeed, there is a double real solution for \(\alpha > 2\epsilon\) if

\[
(2\epsilon)^2 [g (1 + \alpha) + U]^2 + [(2\epsilon)^2 - \alpha^2] (1 + \alpha)^2 = 0;
\]

(H.3)

which corresponds to

\[
U = (1 + \alpha) \left[-g \pm \frac{\sqrt{\alpha^2 - (2\epsilon)^2}}{2\epsilon}\right].
\]

(H.4)

Apart from being real in contrast to imaginary, a solution for the dimensionless impurity diamagnetic flow should be non-negative to be physical. From (6.11), at least one solution is \(D = 0\) if

\[
g^2 (2\epsilon)^2 - (1 + \alpha)^2 - (g + U)^2 = 0.
\]

This takes place when

\[
U = -g \pm \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2},
\]

(H.5)

which is defined for \(|g| \geq \frac{1 + \alpha}{2\epsilon}\).

At that point, at least one of the two solutions changes sign. Both of them change sign simultaneously if the solution is double, satisfying (H.4) and (H.5) at the same time for \(\alpha > 2\epsilon\) and \(|g| \geq \frac{1 + \alpha}{2\epsilon}\). The smallest \(U\) for which a double solution is obtained corresponds to \(D = 0\) if

\[
\alpha g \pm \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2} = \alpha g - \frac{1 + \alpha}{2\epsilon} \sqrt{\alpha^2 - (2\epsilon)^2}.
\]

This expression can be squared

\[
g^2 (2\epsilon)^2 - (1 + \alpha)^2 = \alpha^2 g^2 + \frac{(1 + \alpha)^2 \left[\alpha^2 - (2\epsilon)^2\right]}{(2\epsilon)^2} + 2\alpha g \frac{1 + \alpha}{2\epsilon} \sqrt{\alpha^2 - (2\epsilon)^2}
\]
and solved for $g$ to find

$$g = -\frac{\alpha}{\sqrt{\alpha^2 - (2\epsilon)^2}} \frac{1 + \alpha}{2\epsilon}.$$  

Analogously, the larger $U$ for which a double solution is obtained corresponds to $D = 0$ if

$$\nabla g \pm \sqrt{g^2 (2\epsilon)^2 - (1 + \alpha)^2} = \nabla g - \alpha g + \frac{1 + \alpha}{2\epsilon}, \sqrt{\alpha^2 - (2\epsilon)^2}$$

which corresponds to

$$g = \frac{\alpha}{\sqrt{\alpha^2 - (2\epsilon)^2}} \frac{1 + \alpha}{2\epsilon}.$$  

For very large $U$ in magnitude, the values of the dimensionless impurity diamagnetic flow approaches

$$\lim_{|U| \to \infty} D = \lim_{|U| \to \infty} \frac{\alpha U \pm 2\epsilon |U|}{(2\epsilon)^2 - \alpha^2}.$$  

(H.6)

On the one hand, both roots in (6.12) have the same limit for $\alpha > 2\epsilon$ given by

$$\lim_{U \to -\infty} D \to +\infty$$  

(H.7)

and

$$\lim_{U \to +\infty} D \to -\infty.$$  

(H.8)

On the other hand, for $\alpha < 2\epsilon$, the roots corresponding to the $+$ sign $D_+$ and $-$ sign $D_-$ in (6.12) behave differently as $U$ gets larger in magnitude; namely

$$\lim_{|U| \to \infty} D_+ \to +\infty$$  

(H.9)

and

$$\lim_{|U| \to \infty} D_- \to -\infty.$$  

(H.10)

From this analysis, the regions in $g$ and $U$ space with physical $D$ are derived and sketched in Table H.2.
<table>
<thead>
<tr>
<th>$\alpha$ domain</th>
<th>$g$ domain</th>
<th>Regions in $U$ space where $D$ is positive</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g \leq -\frac{1+\alpha}{2\epsilon}$</td>
<td>Positive root</td>
<td>$U_{D0-} = -g - \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$, $U_{D0+} = -g + \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$</td>
</tr>
<tr>
<td>$-\frac{1+\alpha}{2\epsilon} &lt; g \leq \frac{1+\alpha}{2\epsilon}$</td>
<td>Positive root</td>
<td>$U_{D0-} = -g - \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$, $U_{D0+} = -g + \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$</td>
</tr>
<tr>
<td>$\frac{1+\alpha}{2\epsilon} &lt; g$</td>
<td>Positive root</td>
<td>$U_{D0-} = -g - \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$, $U_{D0+} = -g + \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$</td>
</tr>
<tr>
<td>$g \leq -\frac{\alpha(1+\alpha)}{2\epsilon \sqrt{\alpha^2 - (2\epsilon)^2}}$</td>
<td>Negative root</td>
<td>$U_{D0-} = -g - \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$, $U_{D0+} = -g + \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$</td>
</tr>
<tr>
<td>$-\frac{\alpha(1+\alpha)}{2\epsilon \sqrt{\alpha^2 - (2\epsilon)^2}} &lt; g \leq -\frac{1+\alpha}{2\epsilon}$</td>
<td>Negative root</td>
<td>$U_{D0-} = -g - \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$, $U_{D0+} = -g + \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$</td>
</tr>
<tr>
<td>$-\frac{1+\alpha}{2\epsilon} &lt; g \leq \frac{1+\alpha}{2\epsilon}$</td>
<td>Negative root</td>
<td>$U_{D0-} = -g - \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$, $U_{D0+} = -g + \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$</td>
</tr>
<tr>
<td>$\frac{1+\alpha}{2\epsilon} &lt; g$</td>
<td>Negative root</td>
<td>$U_{D0-} = -g - \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$, $U_{D0+} = -g + \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$</td>
</tr>
<tr>
<td>$\frac{\alpha(1+\alpha)}{2\epsilon \sqrt{\alpha^2 - (2\epsilon)^2}} &lt; g$</td>
<td>Negative root</td>
<td>$U_{D0-} = -g - \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$, $U_{D0+} = -g + \sqrt{g^2(2\alpha)^2 - (1 + \alpha)^2}$</td>
</tr>
</tbody>
</table>

**Table H.2:** Roots of (6.12) with physical impurity diamagnetic flow and zero impurity density at some poloidal angle for $\alpha \neq 2\epsilon$. 

**APPENDIX H. IN-OUT ASYMMETRY BOUNDARIES**
Appendix I

Maximum in-out asymmetry

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I.2 Number of $D$ roots by studying monotonicity and limits at large $|U|$ .................. 194
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APPENDIX I. MAXIMUM IN-OUT ASYMMETRY

I.1 Symmetries

The following relations can be deduced from (6.15):

\[ D_+ [\alpha, g, U] = -D_- [\alpha, -g, -U] \]  \hspace{1cm} (I.1)

and

\[ (D_+ - g) [\alpha, U + g (1 + \alpha)] = - (D_- - g) [\alpha, - (U + g (1 + \alpha))] \]

\[ = \frac{1 + \alpha}{\alpha} \left[ -1 + \frac{(1 + \alpha)^2}{g (1 + \alpha) + U} \left( 1 + \frac{1 + \alpha}{g (1 + \alpha) + U} \right)^2 \right] \]  \hspace{1cm} (I.2)

I.2 Number of $D$ roots by studying monotonicity and limits at large $|U|$

The solutions provided in (6.15) are only physical for non-negative values of the diamagnetic effect coefficient $D$. In order to determine the maximum number of roots that (6.15) may have, attention is drawn to its monotonicity. The derivative of the smaller root $D_-$ with respect to $U + g (1 + \alpha)$ is

\[ \frac{\partial (D_- - g)}{\partial [U + g (1 + \alpha)]} = \frac{1}{\alpha} \left[ -1 + \frac{(1 + \alpha)^2}{g (1 + \alpha) + U} \left( 1 + \frac{1 + \alpha}{g (1 + \alpha) + U} \right)^2 \right] \]  \hspace{1cm} (I.3)

This derivative only changes sign outside of $U < -g (1 + \alpha)$, the domain where the maximum in-out asymmetry correspond to $D_-$ according to (6.16), since

\[ \frac{\partial (D_- - g)}{\partial [U + g (1 + \alpha)]} = 0, \text{ for } U + g (1 + \alpha) = (1 + \alpha) \sqrt{\frac{1 + \sqrt{5}}{2}} > 0. \]

Thus, $D_-$ is monotonously decreasing for $U + g (1 + \alpha) < 0$, because

\[ \lim_{g (1 + \alpha) + U \to -\infty} \frac{\partial (D_- - g)}{\partial [U + g (1 + \alpha)]} = -\frac{1}{\alpha} < 0. \]
Due to the symmetry pointed out in (I.2), the derivative of the larger root \( D_+ \) with respect to \( U + g \,(1 + \alpha) \) satisfies
\[
\frac{\partial (D_+ - g)}{\partial [U + g \,(1 + \alpha)]} \bigg|_{U+g(1+\alpha)} = \frac{\partial (D_- - g)}{\partial [U + g \,(1 + \alpha)]} \bigg|_{-U+g(1+\alpha)}.
\] (I.4)

Consequently, \( D_+ \) is also monotonously decreasing with \( U + g \,(1 + \alpha) \) in the domain where it corresponds to a maximum in the impurity density in-out asymmetry, \( U + g \,(1 + \alpha) \geq 0 \).

In conclusion, the value of \( D \) corresponding to a maximum impurity density in-out asymmetry in the experimentally observed direction is not only continuous but also monotonously decreasing. In conclusion, there is no more than one root, if any at all. The existence of a root in \( D \) or lack of it can be deduced from the values for large positive and negative \( U \),
\[
\lim_{U \to -\infty} D_- \to \lim_{U \to -\infty} \frac{-(U + g) - (1 + \alpha)}{\alpha} \to +\infty \quad \text{(I.5)}
\]
and
\[
\lim_{U \to +\infty} D_+ \to \lim_{U \to +\infty} \frac{-(U + g) + (1 + \alpha)}{\alpha} \to -\infty. \quad \text{(I.6)}
\]
Since these limit have different sign, it can be concluded that there is always one root of \( D \), so there is a maximum impurity density in-out asymmetry only for values of \( U \) smaller than that corresponding to the root.

### I.3 Region where the root is located

The region where the root is located can be delimited by imposing \( D = 0 \) in (6.15),
\[
\frac{1 + \alpha}{g \,(1 + \alpha) + U} + \frac{g + U}{1 + \alpha} = \pm \sqrt{\frac{(1 + \alpha)^2 + [g \,(1 + \alpha) + U]^2}{[g \,(1 + \alpha) + U]^2}},
\]
and squaring each of the terms to find
\[
\frac{(1 + \alpha)^2}{[g \,(1 + \alpha) + U]^2} + \frac{2 \,(g + U)}{g \,(1 + \alpha) + U} + \left( \frac{g + U}{1 + \alpha} \right)^2 = \frac{(1 + \alpha)^2 + [g \,(1 + \alpha) + U]^2}{[g \,(1 + \alpha) + U]^2},
\]
which leads to
\[
\left( \frac{g + U}{1 + \alpha} \right)^2 = 1 - 2 \frac{g + U}{g (1 + \alpha) + U}. \tag{I.7}
\]

The LHS of (I.7) is non-negative, so the RHS should be non-negative as well. As a consequence, \( D = 0 \) is contained in the interval where \( U \) is between \(-g (1 - \alpha)\) and \(-g (1 + \alpha)\).
Appendix J

Impurity density in-out asymmetries as a function of effective impurity charge and fluid and kinetic bulk ion effects

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J.2 Two-dimensional model with impurity diamagnetic and radial effects ............................... 198
J.1 One-dimensional model

The impurity density in-out asymmetry captured by the state-of-the-art one-dimensional models \([15]\) can be calculated for the whole range of effective impurity charge \(\alpha\) and fluid \(g\) and kinetic \(U\) bulk ion friction by using (6.4) to find the contours in Fig. J.1.

In Fig. J.1 blue is used for outboard impurity accumulation in contradiction with the experiments, while red is used for the experimentally observed six-fold inboard impurity accumulation. The intermediate color used is yellow, since white is reserved to denote the unphysical regions, given by a non-positive impurity density at some poloidal angle and thus not satisfying (6.8). These unphysical regions are delimited by a purple surface. The region under the green plane indicate where the two-dimensional model captures stronger in-out asymmetries than the one-dimensional models.

J.2 Two-dimensional model with impurity diamagnetic and radial effects

The impurity diamagnetic flow that corresponds to the maximum in-out asymmetry can be found where the first derivative of the latter cancels with negative second derivative or at a physical boundary, as analytically calculated in Sec. 6.4 and Sec. 6.2, respectively. Physical boundaries can be given by the impurity density becoming negative at some poloidal angle or the dimensionless diamagnetic flow coefficient reaching a really large number (see Sec. 6.3) or the one-dimensional value of \(D = 0\). Fig. J.2 shows the contours of strictly positive ‘impurity diamagnetic’ friction corresponding to the closest in-out asymmetry to the experiments, represented in Fig. J.3.
Figure J.1: Contours of impurity density in-out asymmetry obtained without diamagnetic effects.
Figure J.2: Contours of 'impurity diamagnetic' friction corresponding to the closest in-out asymmetry to the experiments.
Figure J.3: Contours of the in-out asymmetry closest to the experiment that the two-dimensional model can capture.
Figure J.4: Comparison of the contours of impurity density in-out asymmetry without ‘impurity diamagnetic’ friction (left) and with the dimensionless ‘impurity diamagnetic’ friction $D$ represented in Fig. 6.3 to get the closest to the experiments (right).
Bibliography


