Collector Probe Measurements of SOL Impurity Accumulation and the Implications of SOL Flows on the Accumulation Amount

Shawn Zamperini
zamp@vols.utk.edu

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David C. Donovan, Major Professor

We have read this dissertation and recommend its acceptance:

David C. Donovan, Lawrence Heilbronn, Peter C. Stangeby, Ezekial A. Unterberg

Accepted for the Council:

Dixie L. Thompson

Vice Provost and Dean of the Graduate School

(Original signatures are on file with official student records.)
Collector Probe Measurements of SOL Impurity Accumulation and the Implications of SOL Flows on the Accumulation Amount

A Dissertation Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Shawn Zamperini
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Dedicated to my mother, who taught me the power of a strong work ethic, and to my father, who taught me how to use my head for something besides a hat rack. To my loving girlfriend, Jessica, who is the most supportive person on the planet, and to the pets in my life: Puck, Rufus and Eve.
None of this would be possible without the guidance of my advisor, David Donovan, or those in my research group who worked alongside me and helped me figure out what I was trying to say. A special thanks to Jonah Duran for being an excellent colleague (and friend!) to work besides these past five years, and to Jacob Nichols for essentially becoming my second advisor. I would also like to mention the detailed back and forth emails with Peter Stangeby, David Elder and Ezekiel Unterberg and how extremely valuable to me they have been. Oftentimes these discussions have been more valuable to me than any paper or textbook could be. Additional thanks to Peter Stangeby for the numerous edits on my papers and for helping me become a better writer. Of course, the biggest of thanks to my parents, Hazel and Mike, without which I would not been born (also thanks for letting me move back home during the final months of this dissertation!). Also, thank you Jessica for emotionally supporting me from start to finish. Finally, I would like to acknowledge COVID-19 in the worst way possible for making the final year of this dissertation so difficult.
Abstract

A collector probe in its simplest form is a rod inserted into a plasma so that impurities are deposited onto it. These probes are then removed and analyzed to determine the deposition profile both along the length of probe and across the width of it. This dissertation covers a series of collector probes experiments and accompanying interpretive modelling all with the main goal of providing evidence for long-hypothesized near scrape-off layer (SOL) accumulation of impurities that can lead to efficient core contamination. The structure of this dissertation is as follows. A brief outline of fusion energy and why we need it is given in Chapter 1. Chapter 2 goes over the basics of the SOL region in tokamaks, as well as the basics of impurity transport and collector probes. A brief history of collector probes is also presented. Chapter 3 presents collector probe results and trends from the DIII-D Metal Rings Campaign. This includes a description of the hardware and software used, a scaling law to determine what led to the most tungsten deposition on the probes, explaining asymmetries between the two probes faces by how far they were from the separatrix, interpretive 3DLIM simulations of deposition patterns that suggest W radially transports via convection in the far-SOL, and that a “simple” SOL prescription in the far-SOL is most appropriate. Chapter 4 presents a deep-dive analysis into two collector probes that were inserted for similar shots differing primarily in the toroidal magnetic field ($B_T$) direction. It is proposed that the differences in the deposition profiles can be explained in the context of a near-SOL impurity accumulation only occurring in a particular $B_T$ direction. In the opposite $B_T$ direction, fast SOL flows may flush out impurities that would otherwise accumulate. This hypothesis is studied via DIVIMP and 3DLIM simulations. Chapter 5 introduces a set of methane injection experiments meant to build upon the results of Chapters 3 and 4, and to provide more convincing evidence of near-SOL accumulation. Preparation that went into the experiments
and preliminary analysis is presented. Possible areas for dedicated analysis are described. Finally, Chapter 6 puts in context the contributions of this dissertation to the wider field of impurity transport in tokamaks before concluding.
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Chapter 1

World energy usage and fusion

1.1 The world’s energy demand

The world is constantly changing; borders between countries are fluid, new leaders take power daily, and today’s technological breakthrough is tomorrow’s technological antique, yet one thing that remains constant is the world’s ever increasing demand for energy. Increasing energy consumption is generally related to a higher quality of life, so there is reason that this trend is not inherently bad. For example, energy consumption per capita trends very strongly with the Social Progress Index (SPI), Fig. 1.1a [28]. The U.S. Energy Information Administration predicts that the world’s energy use will continue to rise, increasing in 2050 to roughly 60% more than what it is today, Fig. 1.1b.

While Fig. 1.1b shows that renewables like solar and wind power will likely remain important in supplying the world’s increasing energy demand, the intermittent nature of them introduces a degree of volatility to the available power; renewables are affected by the unpredictable changes in weather, which will continue to only get more unpredictable as climate change intensifies. The future will require a reliable and consistent form of clean energy, one in which events like droughts and a lack of wind cannot cripple. Nuclear fission is a viable candidate, but it unfortunately suffers from public misconceptions of the dangers involved and thus policy and constructions of new plants is difficult. Furthermore, the current reserves of uranium are only enough to last a little over 200 years [24]. Nuclear fusion offers a path forward.
1.2 Nuclear fusion in tokamaks

The envisioned fuel source for fusion, deuterium (D) and tritium (T), is essentially limitless; deuterium is abundantly found in the oceans and tritium can be bred from lithium. In a D-T fusion reaction, a 3.5 MeV He atom and a 14.1 MeV neutron are released. The energetic neutrons can then be absorbed in a moderating material called a neutron blanket, which generates heat that can be extracted via the steam cycle. This is the process targeted by the multinational ITER experiment under construction in France.

Current development on fusion is focused on tokamaks, like ITER. A tokamak is a donut-shaped vacuum vessel which contains a plasma that can be upwards of 10 million degrees Celsius (around 10 keV, the optimum temperature for D-T fusion). A schematic of ITER is shown in Fig. 1.2. The vessel that holds the plasma is shown in orange, with all the necessary diagnostics and systems surrounding it. The plasma is suspended in the vacuum vessel with strong magnetic fields (about 11 T) to limit plasma contact with the walls, though it is unavoidable to completely limit all contact. For this reason, the primary region of plasma surface interaction is in the divertor (the white region around the bottom of the vessel). Magnetic fields intentionally direct the plasma that escapes the core towards this highly resistant to plasma damage area. While divertors offer a significant improvement in keeping impurities, i.e. anything that is not deuterium or tritium, out of the main plasma, it is inevitable that some form of core plasma contamination will occur. For example, sputtered particles from the divertor and wall can transport through the plasma, as either neutrals or ions, and into the core, and the byproduct of D-T fusion is helium, which is an impurity as well.

One of the main reasons we care so much about impurities and keeping them out of the plasma is that they can radiate away a large portion of energy needed to heat the plasma. The ITER divertor will be made out of tungsten since it has the highest melting point of any material, but unfortunately it can be shown that the radiated power by an impurity in a plasma scales with the square of its atomic charge, \( Z^2 \) [53]. Thus, tungsten is one of the worst radiators there is. Typically the total amount of tungsten allowed in the core before what is called a radiative collapse happens is on the order of a fraction of a percent of the
Figure 1.1: (a) SPI vs. energy consumption shows increased energy consumption correlates with a higher quality of life. (b) Projected world energy use up to 2050.

Figure 1.2: Reconstruction of what the ITER tokamak will look like. The actual vacuum vessel is shown in orange.
total plasma content. Understanding the path impurities follow, say from the divertor into the core plasma, is a paramount issue in today’s fusion research. Only once we understand these transport pathways that impurities take can we then solve the issue of core impurity contamination.

This paper focuses on impurity transport in the context of collector probe experiments. Chapter 2 will cover a literature review of the current state of knowledge of impurity transport and what past collector probe experiments experiments have discovered. Chapter 3 will go over recent collector experiments on DIII-D during the Metal Rings Campaign I (MRC) and recent modeling efforts using a revitalized code called 3DLIM. Chapter 4 presents a deep-dive analysis on two collectors probes inserted for similar shots differing primarily in toroidal field direction. It is hypothesized that a near-SOL impurity accumulation may exist only in a particular field direction. Chapter 5 introduces a set of methane injection experiments with the goal of expounding upon the results of Chapter 4. Finally, Chapter 5 present opportunities for future areas of research and places the results of this dissertation in the context of the wider field of impurity transport in tokamaks.
Chapter 2

Impurity transport and collector probes

2.1 The tokamak scrape-off layer

The plasma in a tokamak can effectively be divided up into two sections: the core plasma, and the scrape-off layer (SOL). The core is where all the fusion reactions occur and temperatures of 10 keV can be found. The SOL is the area between the core plasma and the walls of the device, and temperatures are typically in the 1-100 eV range. The line which divides the two regions is called the separatrix. A cross section of the DIII-D tokamak is shown in Fig. 2.1. The lines are magnetic field lines, and since plasma is confined by magnetic fields, they also represent the shape of the plasma. The dotted lines are the core of the plasma, the solid lines are the SOL region, while the thick solid line separating the two regions is called the separatrix. The structure surrounding the field lines are the vessel wall. This paper will only focus on the SOL region of the plasma, and will not go into detail on the core plasma physics (which is surprisingly rather different from SOL physics). A note on coordinates: the primary coordinates used in tokamaks are radial (outward from the center of the core), poloidal (in the approximately circular direction on the page) and toroidal (into the page and around the donut shaped device).

The SOL is a very complex shape, and analyzing it as such would be extremely difficult, so we must make a set of assumptions to simplify understanding it. This brings us to two
of the most important powerful simplifications one can make of the SOL: toroidal symmetry and the idea of "straightening out" the SOL.

Toroidal symmetry assumes that the location of the cross section is indifferent to the toroidal location of it, so in effect one reduces the problem from a 3D one (radial, poloidal and toroidal) to a 2D one (radial and poloidal). This simplification is based on the fact that the toroidal velocity of the plasma is extremely fast, and that any toroidal variation in the plasma is rapidly transported around the entire device, rendering it essentially toroidally symmetric.

The idea of straightening out the SOL is covered in one of the primary texts of SOL physics by Stangeby [53], and will be briefly reviewed here. Imagine grabbing the solid lines in Fig. 2.1 and peeling them off, then laying them down straight. One would end up with Fig. 2.2. The left and right border are the divertor targets, the top is the core plasma, while the bottom is the wall of the device. The variable L is called the connection length, which represent half the distance between the two divertor targets. Since the magnetic field lines have been straightened out, we can rename our coordinate system as radial and parallel to the magnetic field lines (left to right). This significant simplification allows us to work in a Cartesian like coordinate system. Decades of experience have shown these two simplifications to be rather accurate in explaining SOL physics.

One of the primary research topics of SOL physics is understanding the spatial distributions of plasma temperature, density or velocity, to name a few variables. The SOL is relatively not well diagnosed in modern day tokamaks, and interpretation of SOL measurements can be difficult, [33, 56, 61] to cite a few examples, see the book by Ian Hutchinson for an extensive review of plasma diagnostics [32]. These plasma variables, or the background plasma, are crucial in understanding impurity transport in the SOL. When modelling the SOL using codes such as DIVIMP (chapter 3 and 4), a form of interpretive modelling is done where the results of the experiment are replicated in the code to figure out what the plasma conditions were (examples in [54] and chapter 4). This is in contrast to predictive modelling with codes like SOLPS-ITER [69], where the modelling can be done before the experiment in an attempt to predict what will happen.
Figure 2.1: Cross section of the DIII-D tokamak operated by General Atomics. Solid lines are the SOL region, dotted lines are the core plasma. The thick black line separating the two is the separatrix.

Figure 2.2: The straightened out SOL. The top represents the core, or main plasma. The left and right targets represent the divertor regions. The wall is the bottom.
Despite not being well diagnosed, the SOL can primarily be divided up into two regimes: conduction-limited or sheath-limited. The primary distinguishing characteristics between the two regimes is the existence of parallel temperature gradients. Specifically, the conduction-limited SOL can contain significant parallel temperature gradients that result in lower temperatures at the target. The sheath-limited regime is defined by no gradients, and thus a constant plasma temperature along the field line. From an operating perspective, conduction-limited is desirable since low target temperatures mean less sputtering and less damage to plasma facing materials (PFCs), though at the trade off of being significantly more complex to understand. Sheath-limited is conceptually more simple to understand. This explains the alternate names these regimes go by, the complex and simple SOL regimes.

As mentioned before, a sheath-limited regime is characterized by constant plasma temperature along a field line, though radially it can be approximated to decrease exponentially. An example of what a sheath-limited SOL may look like is shown in Fig. 2.3. These graphs can just be imagined as the same as Fig. 2.2, just with the temperature or density contours filled in. These plots exclude variations due to the plasma sheath, which is an area on the order of less than a mm. The sheath acts to accelerate ions, while repelling electrons, to the solid surface. This would result in a decrease of plasma density near the sheath, among other effects. Without going into details, the sheath has a penetrating effect throughout most the SOL that can influence the forces on particles. This is the namesake for this regime, namely that the sheath is ultimately what controls the transport of particles in this SOL regime.

The conduction-limited SOL is significantly more complex, and comes in many different shapes and sizes. Selecting the correct conduction-limited SOL in models is a difficult process, and often relies on interpretive modeling to determine. One possible shape of a conduction-limited SOL is shown in Fig. 2.4. The key defining characteristic of the conduction-limited SOL is the existence of parallel temperature gradients, owing to the finite heat conductivity of the plasma. Thus we see the namesake of this regime, namely that heat conduction is the main controlling factor in the transport of particles in this SOL. There are also a number of other controlling quantities only present in the the conduction-limited SOL. Hydrogen saturated surfaces will release, or recycle, neutral hydrogen back into
the plasma, which will ultimately ionize and thus provide a cooling effect (ionization near the target is one reason the conduction-limited SOL can achieve low target temperatures). Another example is volume recombination at very low temperatures (<1 eV). This is when the temperature is low enough for the plasma ions to recombine into neutrals, which acts as another cooling effect (this is very important for divertor detachment, which is a regime ITER must operate in, but out of the scope of this dissertation). There are many other equally important controlling factors in the conduction limited SOL, but the takeaway here is that the trade off for lower target temperatures is that there are significantly more knobs to turn.

2.2 The impurity chain

The topic of SOL physics and what the profiles of these various parameters look like could fill an entire book (indeed a very large one, see [53]), but that is not the goal of this dissertation. The topic here is a subset of SOL physics called impurity transport. Defined simply, an impurity is anything in the plasma that differs from the background plasma, which is typically deuterium. Some common impurities include helium from the DT fusion reaction, carbon from the walls, tungsten from the divertor, or intentionally injected impurities like neon (impurities with enough electrons radiate, making them easier to track through the plasma). Generally speaking, impurities are bad for plasma performance. They have more electrons than the fully stripped hydrogen, and thus can radiate away energy as photons, cooling the plasma. The core plasma requires high temperatures, and impurities are surprisingly efficient at lowering those temperatures. For example, if the core plasma consisted of about 10% carbon, it would radiate away about 10% of the fusion power generated. For the case of tungsten, on the order of only 0.01% tungsten concentration would radiate away 10% of the fusion power generated [68]. Clearly, these are unacceptable losses, and can lead to a phenomena called a radiative collapse, which is when the plasma starts to uncontrollably radiate away energy leading to a disruption. Impurities can also be beneficial though, such as injecting nitrogen near the divertor to facilitate detachment. Though if nitrogen leaks out of the divertor region and reaches the core the aforementioned harmful effects apply.
Figure 2.3: An example of the plasma temperature (Te, left) and density (ne, right) in a sheath-limited SOL.

Figure 2.4: An example of the plasma temperature and density in a conduction-limited SOL. Note the parallel temperature gradient, and increasing density at the targets.

Figure 2.5: The impurity chain involving sourcing from the divertor, transport through the SOL, and core contamination.
A key thrust is therefore to restrict impurities from reaching the core, and to do this we must understand the path they take from their point of origin to the core. This is conveniently broken up into three steps: sourcing, transport, contamination (Fig. 2.5 [62]). Sourcing, for example in Fig 2.5, involves impurities sputtered from the divertor. These impurities are ionized at some distance, which is when they begin to experience the forces and flows of the SOL plasma. Once the impurities are ionized, they go into the next step of SOL transport. In the SOL there are a number of forces felt by the impurity ions (more on this in chapter 2.3), that move the impurities around the SOL. This includes forces that could push the impurities back to or away from the targets, or diffusive and/or convective transport that either pushes the impurities outward or inward radially. The inward radially moving particles thus enter the last stage of the impurity chain, core contamination. It is simply not enough to know if an impurity enters the core, but we also need to know where it enters the core. An example of why this needs to be known is some core simulations that study impurities in the core require this input as boundary conditions to their simulations. Understanding the path impurities follow is crucial. Only once we understand this can we begin to meaningfully create plasma scenarios that suppress core contamination.

2.3 Forces on impurities in the SOL

An ionized impurity in the SOL experiences a variety of forces, but generally we start by considering only five main forces parallel to the magnetic field lines as laid out in [53]. These forces can be written out as

\[
F_z = -\frac{1}{n_z} \frac{dp_z}{ds} + m_z \frac{v_i - v_z}{\tau_z} + Z e E + \alpha_e \frac{d(kT_e)}{ds} + \beta_i \frac{d(kT_i)}{ds}.
\]

(2.1)

From left to right the terms describe the impurity pressure gradient force (FPG), the friction force (FF), the electrostatic force (FE), the electron temperature gradient force (FeG) and the ion temperature gradient force (FiG). The variable \(s\) is a field-aligned coordinate parallel to \(B\), such that derivatives in those variables are in regards to how that variable changes along the field line. The variables in each term are:
• **FPG**: $n_z$ is the impurity density and $dp_z/ds$ is the impurity pressure gradient.

• **FF**: $m_z$ is the mass of the impurity, and $v_i$ and $v_z$ are the velocities of the fuel ions and impurities, respectively.

• **FE**: $Z$ is the charge of the impurity and $E$ is the electric field.

• **FeG**: $\alpha_e$ is a coefficient proportional to $Z^2$ and $d(kT_e)/ds$ is the electron temperature gradient.

• **FiG**: $\beta_i$ is a coefficient proportional to $Z^2$ and $d(kT_i)/ds$ is the ion temperature gradient.

Each of these forces are parallel to the field line, and do not have any cross field aspect to them. Cross field transport is generally assumed to be some kind of anomalous diffusion, represented by a diffusion coefficient $D_\perp$, though an analysis in Ch 3.3.4 will suggest a convective treatment is more appropriate, at least in the far-SOL. The direction of these forces along a field line are shown in Fig. 2.6 (taken from Fig. 6.11 in [53]). The FF and FE generally point towards the target, while the FiG and FeG generally point away. The FF and FiG have larger arrows to represent they’re generally the two most dominating forces, so it is those two we will focus on in this discussion. It may be surprising that the FiG force acts to push impurities up the temperature gradient, though this can be explained in the context of the collisions impurities experience with the background plasma. The collision frequency between ions and impurities is inversely proportional to $T_i$, $v_{iz} \sim T_i^{-3/2}$. Thus the impurities experience more frequent collisions with colder ions, and less with hotter ions, moving impurities into regions of higher $T_i$, or up the temperature gradient.

If the FiG is pointing away from the targets on both sides of the SOL, then theoretically there would be a region in the middle where the forces overlap and cancel each other out, creating a stagnation region of about zero net force. Thus, theoretically an accumulation of impurities near the middle of the SOL could potentially form. This *impurity accumulation* is conceptualized in the 2D SOL cartoon of Fig. 2.7. The left and right bounds represent the inner and outer targets, respectively, while the top and bottom represent the core boundary and outer wall. The purple region represents the near-SOL, while the green the far-SOL. Arbitrary impurity sources are imposed in the near-SOL in red, and red arrows demonstrate
the transport of impurities. Here only the two primary forces, FiG and FF, are considered. In the near-SOL, \( T_i \) gradients are significant, and thus the FiG force pushes impurities up the gradient from each target. In the middle where these forces meet and \( T_i \) peaks (\( T_i \) gradient = 0) the impurities could accumulate. The accumulation is depleted only by perpendicular transport, either by contaminating the core or travelling into the far-SOL. In the far-SOL \( T_i \) gradients become less significant and thus the FF may take over as the dominant force. In the simplest scenario, the FF is directed towards the nearest target, but in practice complicated flow patterns can exist. One may also note that we have divided the SOL up into a near and far region, and are only considering the effect of a single force in each. In practice, one must consider both the FiG and FF in the near-SOL as both can be significant. In the far-SOL it is more appropriate to only consider the FF, but it must be noted that all the forces of Eq. 2.3 still apply, and scenarios could exist where the neglected forces end up being non-negligible.

This impurity accumulation is one of the primary motivations for this collector probe study. It has never been directly measured, and this simplified scenario neglects other very important aspect of the SOL that almost certainly affects under what conditions an accumulation could form, and what the actual location of it could be. Examples of this include \( B_T \) dependent parallel flows (chapter 2.3.1) and ExB drifts in the poloidal and radial directions.

### 2.3.1 Influence of parallel SOL flow patterns on the friction force

As evident in Eq. 2.3, the friction force depends on the background plasma velocity, \( v_i \), which as we will show depends on the \( B_T \) direction. In the SOL, plasma flow parallel to field lines is typically reported as a fraction of the sound speed. The sound speed, \( c_s \), is given by:

\[
  c_s = \sqrt{\frac{T_e + T_i}{m_D}}.
\]  

(2.2)

\( T_e \) and \( T_i \) are the electron and ion temperatures given in eV, and \( m_D \) is the mass of deuterium given in eV/\( c^2 \). The fraction of the sound speed is called the parallel Mach number, and is given by \( M_{||} = v_i/c_s \). This ratio is measured with a suitably named Mach probe (see
Figure 2.6: The main forces on impurities in the SOL, and the relative directions and magnitude. FF and FiG typically dominate.

Figure 2.7: Cartoon of how a near-SOL impurity accumulation may form due to the FiG force.
chapter 3.3.4 in [32] for the theory behind them) that plunges into and out of the plasma to provide radial profiles of $M_{||}$. Mach probes often include additional Langmuir probes to provide radial profiles of $n_e$ and $T_e$ as well, which then allow calculating $c_s$ and therefore $v_i$.

An example of Mach probe measurements taken on DIII-D is shown in Fig. 2.8. This plot shows the Mach number for deuterium ($M_{||}D^+$) plotted against distance from the separatrix for both $B_T$ directions. In this plot, a positive Mach number indicates flows towards the outer target (low-field side, LFS), while a negative value indicates flow towards the inner divertor (high-field side, HFS). The location of the Mach probe is at what is called the crown region of the plasma, shown in the inset at the top right. In the USN-$V_{\nabla B_L}$ direction, also called the unfavorable or $B_x\nabla B \downarrow$ or $B_x\nabla B$ towards the divertor direction, the flow in the crown is mostly stagnant ($M_{||} \approx 0$). In the other direction though (USN-$V_{\nabla B_L}$ or favorable or $B_x\nabla B \uparrow$ or $B_x\nabla B$ away the divertor), the flow is on the order of $M_{||} \approx 0.5$ towards the inner target. Note: We will maintain the favorable/unfavorable naming convention going forward due to their simplicity. They are named according to how favorable it is to achieve H-mode in each direction. The L-H transition threshold is not the topic of this dissertation, but we adopt this convenient naming convention regardless.

This observation of fast inner target flows in the favorable $B_T$ direction is not unique to DIII-D, and indeed is observed on most major tokamaks, at least during L-mode experiments [3] [6] [40]. The general pattern is shown in Fig. 2.9. In the favorable $B_T$ direction, flow typically stagnates somewhere below the outboard midplane (OMP) but above the X-point, with fast inner target flows existing throughout most the SOL. In the unfavorable $B_T$ direction, flow stagnates somewhere near the crown with flows directed towards each respective target as one moves away from the crown.

The origin of these parallel flow patterns is still not completely understood, though theories have been put forth. An explanation is likely a combination of multiple physics aspects, such as but not limited to: Pfirsh-Schluter flows [12], ExB drift return flows [12], intrinsic edge momentum [7] and ballooning transport [36]. Irrespective of their origins, the flows patterns can be expected to exist in some capacity in L-mode shots and thus will warrant an investigation into their possible effects.
Figure 2.8: Radial profiles of the parallel Mach number taken during a DIII-D discharge in the crown region for each $B_T$ direction. Fig. from [29].
Figure 2.9: General pattern of parallel SOL flows for each $B_T$ direction as measured on different tokamaks. A positive value indicates flow towards the inner or HFS target. $B_x \nabla B \uparrow$ (red) = unfavorable, $B_x \nabla B \downarrow$ (blue) = favorable. Figure from [6].
The shape of the parallel flow patterns can be thought of as the shape of the friction force and indicates which direction it faces, either towards or away from a particular target. As we will later shown in chapter 4, the poloidal distribution of impurities in the SOL may sensitively depend on the parallel flow pattern and may dictate if near-SOL accumulation occurs or not.

2.4 Basics of collector probes

The primary diagnostic studied here is the collector probe. A collector probe, in its most basic form, is simply just a rod stuck into the plasma. Impurities deposit on the rod, which is then analyzed post-mortem using ion beam analysis techniques, like Rutherford backscattering (RBS), to determine the amount and distributions of impurities on the probe. Collector probes have been used periodically since the late 70’s. Some of the foundational probe experiments can be found in [14, 66, 60, 56], while more modern experiments can be found in [51, 47, 16, 71, 72, 17, 64]. A picture of the some of the probes used in this dissertation is shown in Fig. 2.10. This actually shows three different collector probes of diameters 0.5, 1.0 and 3.0 cm. The collection regions are on both sides of the probe.

An example RBS profile of a collector probe can be seen in Fig. 2.11. The tungsten areal density is plotted against a commonly used parameter called R-Rsep OMP, which is another way of saying how far away that particular point on the probe was from the separatrix (see App. A for a detailed method in mapping a probe location to distance from the separatrix). The two lines, ITF and OTF, represent the two sides of a single probe (ITF/OTF is the naming convention we chose, what the names mean will be explained later). This plot, as do all the other collector probe plots, shows that the amount of tungsten in the plasma increases the closer to the separatrix one gets. The asymmetries between the two sides, or conversely if two sides are symmetric as this one is, can tell us information about the poloidal distribution of impurities in the SOL.

The reason for choosing different sized probes is based on the simple equation,

\[ L_{\text{coll}} = \frac{d^2c_s}{4D_\perp} \]  

(2.3)
Figure 2.10: Set of three different sized collector probes used in the 2016 DIII-D Metal Rings Campaign I.

Figure 2.11: RBS profile of a collector probe inserted in DIII-D. R-Rsep omp is simply the distance of that point on the probe from the separatrix.
$L_{\text{coll}}$ is the *collection* length of the probe. This is a rough approximation of how far along a magnetic field line it gather impurities. $d$ is the diameter of the probe, $D_\perp$ is the perpendicular (or radial) anomalous diffusion coefficient and $c_s$ is the plasma sound speed.

To put numbers to all these variables, a typical temperature for a collector probe may be around $T_e = 10eV$ (note $T_i = T_e$ is often assumed), and $D_\perp \approx 1 \text{ m}^2/\text{s}$. This gives a sound speed of about 44,000 m/s. Thus, for our 0.5, 1.0 and 3.0 cm probes, we have collection lengths of about 0.3, 1 and 10 m along the field line. There are limits though as to how high $L_{\text{coll}}$ can actually be. To understand, let’s look at a plot of what the plasma velocities in the far-SOL, with and without a probe inserted, may look like. In Fig. 2.12, we have two graphs of the plasma velocity, where red indicates a right going velocity, and blue left going. Note this neglects any $B_T$ dependent flow patterns, such as those in chapter 2.3.1, but this simplification may be appropriate due to weak drifts and gradients in the far-SOL. The top is the normal undisturbed plasma, while the bottom is with a collector probe inserted in the middle at parallel = 0. A simple SOL approximation is that the plasma velocity is accelerated to the two targets due to their sink action on the plasma, with a stagnation point in the middle; this is shown in the top graph. The bottom graph is what may happen with a collector probe inserted into the middle. The idea is that each probe face acts as a target/sink, and in effect creating a “mini SOL” between that face and the target it faces. Thus, we see that a stagnation point could exist on each side of the probe.

So what does this have to do with the collection length? The probe can only collect plasma/impurities that are flowing towards it; if the impurity is heading in the other direction, it’s going to deposit on the target. Thus the collector probe can only collect impurities up until the stagnation point that may exist between its face and the target. Put in more technical terms, the probe’s actual collection length, or the *sampling length*, is the smaller value of either its collection length or half the distance to the nearest surface. We denote this $L_{\text{samp}}$. In Fig. 2.13 we demonstrate this effect along the length of each probe type (probes A, B and C correspond to the 3, 1 and 0.5 cm diameter probes, respectively). Fig. 2.13a shows the calculated $L_{\text{coll}}$, which is the same for both the ITF and OTF sides, along with $L_{\text{conn}}$ for each direction. The bottom shows the effective $L_{\text{samp}}$, where $L_{\text{samp}} = L_{\text{coll}}$ if $L_{\text{coll}} < L_{\text{conn}}$ else $L_{\text{samp}} = L_{\text{conn}}$ if $L_{\text{coll}} > L_{\text{conn}}$. For the A probe as seen in Fig.
2.13b, both the ITF and OTF $L_{samp}$ is entirely set by $L_{conn}$ except beyond R-Rsep <5 cm, but probes were never inserted beyond about R-Rsep 7 cm. For the B and C probes, $L_{coll}$ was always smaller than $L_{conn}$ due to the smaller diameters, and thus their $L_{samp}$ are set by $L_{coll}$, at least up until about R-Rsep = 11 cm. Here $L_{conn}$ decreases to very small values due to limiting on portions of the outer wall.

In summary, the motivation for having multiple sized probes is to have a range of different sampling lengths. At this point a valid question would be why do we care about different sampling lengths? The idea behind it is that the largest probe would sample a longer distance along the field line, ideally into the region of impurity accumulation. The smaller probes would then sample the accumulation only partially or not at all. The comparison between the probes would then offer evidence of near-SOL impurity accumulation. This is easier said than done though. In practice one needs to insert the probes to the near-SOL, which may not be possible due to the high temperatures and heat flux. This also includes inserting the probes sufficiently far enough into the SOL such that it is not on field lines that limit on portions of the outer wall. In the experiments of chapter 3 these criteria were not met, though the accompanying analysis in chapter 3 and 4 demonstrates there is still plenty of information contained in the deposition profiles.

2.5 Previous collector probe experiments

To give a sense of what a collector probe experiment looks like, we will go over three older experiments and show what their key results looked like. A key takeaway is that there is not a “one design fits all” collector probe, and just about every experiment utilized a different shaped probe. Some even had the capability to have time resolved measurements of impurity fluxes to the probe during the course of a plasma shot. Another takeaway is that collector probes have been used for decades to measure different kinds of impurities in the SOL, though integration with modelling has never been too extensive (likely due to the fact many codes did not exist during some of these older experiments!).

One of the earliest collector probe experiments was done by McCracken in 1978 [39], Fig. 2.14. Here a rotating disc was used that was exposed to the plasma through a aperture.
Figure 2.12: Velocity plots of SOL plasma. Top: undisturbed plasma with a stagnation point halfway between the two targets. Bottom: disturbed plasma with a collector probe inserted at parallel = 0. Stagnation points form between each face of the probe and the corresponding target it faces.

Figure 2.13: Top: Collection length and the ITF and OTF connection lengths for an A probe. Bottom: The resulting sampling lengths of each probe where $L_{samp} = L_{coll}$ if $L_{coll} < L$, or $L_{samp} = L$ if $L_{coll} > L$. 
This meant that each location along the disc was representative of the impurity flux to the disc during a specific point in time. They measured impurity concentrations at each point on the disc using Rutherford backscattering (RBS), results shown in the right of Fig. 2.14. The solid and dashed lines represent measurements at two different exposure times during a plasma shot for three different impurities (Mo, SS and Ti). The general trend here is the closer to the main plasma the probe is, the more impurity content is measured. This may not be too surprising that the impurities are where the plasma is, but it does give a good baseline of what kind of trends to expect in these measurements.

A later experiment was done in 1982 by Staudenmaier [60]. They exposed a 0.5cm wide probe into the ASDEX tokamak and then removed them and analyzed them using secondary ion mass spectrometry (SIMS), atomic emission spectroscopy (AES), nuclear reaction analysis (NRA) and RBS. A key finding in their work was that the impurity profiles along the probes had two different e-folding lengths as one went radially outward, which is to say the profile decayed exponentially radially with different exponential decay rates between the tip and back of the probes, Fig. 2.15. This figure shows radial profiles (note the log scale) of different impurities measured by SIMS and RBS plotted against the distance from the core plasma (r-a). The explanation presented in this paper for the two different decay rates is a difference in connection lengths for those two parts of the probe due to the presence of a limiter. This pattern would be seen in later collector probe experiments (next paragraph, though with a different explanation), including some of our probes that were inserted into DIII-D (chapter 3).

As a final example of collector probes through the times, we can look at the 2007 experiments of Schustereder [51]. In Fig. 2.16, we see the radial profiles of deuterium, tungsten and iron for a collector probe inserted into ASDEX. Again we see the tungsten profile has a slower decay rate near the tip of the probe (with an eventual falloff at the very tip) compared to the further away section in the range of about 30-40mm. This decrease in decay length though is attributed to sputtering near the tip from iron, as shown by the increased iron content where the tungsten starts to decrease. We call this region near the tip where the tungsten is partially eroded away the re-erosion regime.
Figure 2.14: Left: rotating carbon disc used in the DITE torus to give time resolved impurity measurements. Right: Example impurity measurements at different radial locations along the disc at two different times.

Figure 2.15: Log plot of the radial profiles for probes inserted into the ASDEX tokamak. Note the region closer to the main plasma has a larger decay length than the region further (>11cm).
There are many collector probe papers that have been published in the past few decades, but between roughly 2007-2016, there was a significant decrease. In this time period, codes like DIVIMP and 3DLIM have been significantly developed, and the idea of using these codes to predict or understand collector probe deposition patterns has gained traction, [20]. In the next chapter, we go over the most extensive set of collector probe measurements to date, taken during the DIII-D Metal Rings Campaign. The accompanying modelling with DIVIMP and 3DLIM provides insight into the transport pathways W may take through the SOL, and if the existence of a near-SOL impurity accumulation is compatible with the experimental data. In chapter 5 we review an even more recent set of collector probe experiments that involved injecting isotopic methane into the SOL and detecting it with an array of spectroscopic diagnostics and collector probes. The intent of these experiments was to provide the first direct experimental measurement of near-SOL impurity accumulation.
**Figure 2.16:** Radial profiles of deuterium, tungsten and iron for a collector probe inserted in the ASDEX tokamak. Note the tungsten content begins to decrease when the iron increases, indicating the decrease may be due to iron sputtering away tungsten.
Chapter 3

Collector probes during MRC

Double-sided collector probes (CPs) (see Fig. 2.10), were inserted into DIII-D during the first Metal Rings Campaign (MRC) in summer 2016 [31]. MRC was a multi-faceted campaign with the intent of covering a broad set of impurity sourcing and transport goals. Examples include observing the differences between intra and inter-ELM erosion [70], observing arcing effects along the tiles [11], and applying a heat flux analysis to the metals rings and their survivability [4]. During many of these studies CPs were inserted and thus enabled CP measurements over a wide range of operating conditions. This chapter will cover many of the CP trends and results from MRC. Section 3.1 will go over the CP hardware and the instruments used to obtain CP deposition profiles. Section 3.2 will introduce the codes used to interpret the results. Section 3.3 reviews the observed trends in CP deposition profiles and demonstrates how 3DLIM can explain some of the trends. In particular, section 3.3.2 presents a scaling law for how much W was deposited on CPs, section 3.3.3 presents a more appropriate metric for distance from the separatrix, section 3.3.4 demonstrates how reproducing CP deposition patterns in 3DLIM suggests impurities radially transport via convection instead of diffusion, and section 3.3.5 supports the prescription of a simple SOL background plasma in the very far-SOL.
3.1 Hardware

MRC utilized two isotopically distinct, toroidally symmetric W tiles along the lower divertor as shown in Fig. 3.1. The ring on the shelf consisted of isotopically enriched W (93\% $^{182}$W) while the ring on the floor consisted of natural W (27\% $^{182}$W). Fig. 3.1 also shows the insertion location of the collector probes at the “MiMES” port, which is located at the outside midplane of DIII-D. The two faces are named according to which target they face following the field lines, either inner target facing (ITF) or outer target facing (OTF). The top right figure shows example data taken using the laser ablation inductively-coupled plasma mass spectrometry (LA-ICP-MS, or just LAMS) [17] system at ORNL that was restored for the initial purpose of measuring 2D deposition profiles, i.e. along the length of the probe (as shown) as well as across the faces (not shown). LAMS provides very W measurements on the faces of the CPs at high spatial resolutions.

The Rutherford backscattering (RBS) system at Sandia National Labs was also used to measure W content on the CPs [67]. RBS and LAMS generally were in agreement, as is shown in Fig. 3.2, though the RBS data is not as high resolution. The trade-off is that RBS is a long-established and trusted method, in comparison to the newer LAMS system, so agreement is necessary to give credibility to LAMS measurements.

3.2 Software

A primary goal of the CP experiments was to reproduce the deposition patterns using the codes OSM-EIRENE, DIVIMP and 3DLIM. OSM-EIRENE (or just OSM) is a plasma background solver, while the latter two are Monte-Carlo SOL impurity transport codes. A workflow was developed to manually couple these codes together to give somewhat self-consistent results, Fig. 3.3. The reason for this workflow is that OSM+DIVIMP can only simulate plasmas out to the far-SOL, while 3DLIM is only qualified for use in the very far-SOL. The manual coupling is to bridge the gap between the far and very far-SOL. Additionally, an extensive set of relevant Python scripts were written over the course of this dissertation, and some of the most important are briefly highlighted.
Figure 3.1: Layout of the DIII-D Metal Rings Campaign and relative insertion location of collector probes. The top right plot is example deposition data taken using the LAMS system.

Figure 3.2: Example RBS and LAMS centerline measurements for a collector probe.
DIVIMP is a Monte-Carlo impurity transport code that has undergone continuous development since its origin in the 80’s. It is part of the OEDGE suite of code packages, but it is common to refer to the whole suite as just DIVIMP due to DIVIMP being the most used code. Other codes included in the OEDGE suite are 3DLIM, EIRENE and OSM. All are written in Fortran.

OSM (Onion Skin Model) is used to generate a plasma background by solving the 1D fluid equations (chapter 12 of [53]). The 1D fluid equations for the simplified case of $T_e = T_i$ can be given by:

$$\frac{d}{dx} (nv) = S_p$$  \hspace{1cm} (3.1)

$$\frac{d}{dx} (m_iv^2n + 2kT) = m_iv\sigma\nu_{in}nn$$  \hspace{1cm} (3.2)

$$\frac{d}{dx} \left( \left( \frac{1}{2}m_iv^2 + 5kT \right) nv - \kappa_{0e}\frac{T_e^{5/2}dT_e}{dx} \right) = Q_R + Q_E$$  \hspace{1cm} (3.3)

Eq. 3.1 is the continuity equation, Eq. 3.2 is the momentum equation, and Eq. 3.3 is the energy equation. $x$ is the field aligned coordinate ($s$ in chapter 2.3), $n$ is the plasma density, $v$ is plasma velocity, $S_p$ is the particle source, $m_i$ is the deuterium ion mass, $kT$ is the plasma temperature, $\sigma\nu_{in}$ is the ion neutral collision frequency, $n_n$ is the neutral density, $\kappa_{0e}$ is the electron heat conductivity, $Q_R$ is the collisional heating due to electrons, and $Q_E$ is the energy due to ionization of neutrals. OSM in fact solves a more complicated version of these equations, but the basic formulation is that it self-consistently solves a set of conservation, momentum and energy equation similar to those above.

OSM modelling has been adapted in different ways, each with their own strengths and weaknesses. The three most common methods, designated by a “SOL option”, are SOL22, 23 and 28. In each method, the flux tubes are designated as rings. SOL22 is a Runge-Kutta solver that solves the 1D fluid equations starting from the targets up to the midpoint of a ring. Thus each ring has two solutions, and it falls on the user to iteratively tweak input parameters until the solutions from each side on a ring match provided upstream Thomson scattering $n_e$ and $T_e$ data. Examples of SOL22 in action will be deferred until chapter 4.
SOL23 was created by Fundamenski as part of his dissertation in 1995 [26], and solves the 1D fluid equations for the entire ring instead of the half-ring prescription of SOL22. Instead of generating a solution based off the target data, it generates a solution and it is up to the user to tweak input parameters until the solution matches the target data. An example of SOL23 applied to JET is found in [27]. SOL28 was developed as part of James Harrison’s dissertation [30] under supervision of Steve Lisgo. In SOL28 one specifies poloidal locations where $n_e$, $T_e$ and $T_i$ are known, and then generates a solution that is forced to match the input data by modifying volume source terms in the 1D equations. SOL28 has demonstrated its ability to reproduce detachment, among other things. An example applied to an ITER case study looking at W as a target material is seen in [37]. The primary downfall of SOL23 and SOL28, compared to SOL22, is simply lack of documentation. As of the time of this writing, both SOL23 and SOL28 are unusable as part of the main development branch of OEDGE, and can only practically be used by those who developed them on their own OEDGE branches. SOL22 on the other hand is well-documented and developed as part of the main OEDGE branch, and is thus the one used in this dissertation.

OSM does not explicitly include any drift-dependent effects, though they are implicitly considered by virtue of using experimental target data to generate plasma backgrounds. The experimental data contains all the physics, and by building a solution from the targets thus includes these physics to some degree. By further constraining the upstream measurements to Thomson scattering data, the primary concerns become the data between target and Thomson data. Specifically parameters like the temperature gradients (does it monotonically increase from target to Thomson, or does it increase rapidly near the target and remain relatively flat up until the location of the Thomson data point). This is where the 1D fluid equations “fill in the gap”, which in the simplest of scenarios means applying the 2-point model (chapter 4 of [53]) between the two measurement locations. The 2-point model has been very extensively used and long-proven to be a reliable estimate of parallel $n_e$ and $T_e$ profiles.

EIRENE is a neutral transport code, which is actually maintained as part of the SOLPS-ITER code suite [69]. Among other things, it tracks neutrals until they ionize, which then
are fed into either the fluid equations in OSM as source terms, or into DIVIMP where the ionized neutral may be tracked through the plasma as an impurity ion.

DIVIMP is a versatile code with many options. The standard usage is to supply DIVIMP a plasma background that has already been generated, such as one from OSM or SOLPS, and then launch neutrals or ions into the plasma and follow them until they ultimately deposit on a surface or leave the simulation domain. DIVIMP includes all the forces shown in Eq. 2.3, as well as parallel diffusion and ExB drifts, to calculate transport parallel to the magnetic field. Radially, impurity ions are transported via anomalous diffusion and/or convection, including ExB drifts. The radial transport coefficients for impurities are unknown, so these act as knobs to turn to match experimental measurements, if any exist. DIVIMP simulations have been performed on many tokamaks. Some examples include: Study of methane injection in DIII-D [40], preliminary MRC analysis on DIII-D [20], comparison of DIVIMP results to EDGE2D on JET [35], and transport of W in EAST [73]. An in-depth case study using OSM+DIVIMP+3DLIM is described in section 4.

3.2.2 3DLIM

3DLIM is a Monte Carlo impurity transport code that follows ions similar to that of DIVIMP, except in a 3D context, Fig. 3.4. The coordinate system is parallel to the magnetic field (B), radial (R) and poloidal (P). In Fig. 3.4 a synthetic collector probe has been inserted into the 3D volume, and the flux tubes it intersects are indicated in grey. Absorbing boundaries are used for parallel boundaries and the wall to simulate target deposition. Reflecting boundaries are imposed on the poloidal bounds to restrict the computational domain to just that around the collector probe and is justified as long as the plasma and impurity transport near the reflecting boundaries is unaffected by the probe, a condition easily satisfied with reflecting boundaries about 40 cm apart. In the figure on the right of Fig. 3.4 an arbitrary impurity source region in red has been imposed to demonstrate a typical injection location for impurities.

3DLIM must generate its own background plasma as it lacks the capability of the more advanced OSM options such as SOL22. It can generate either a completely conduction or convection-limited SOL (complex and simple SOL, respectively), and does not iterate with
**Figure 3.3:** Flowchart outlining the OSM+DIVIMP+3DLIM workflow.

**Figure 3.4:** 3D simulation volume of 3DLIM and the boundary conditions imposed. The figure on the right includes a typical impurity injection region in red.
a neutral code such as EIRENE. Thus, it is currently best used in regions far from the separatrix where background plasma factors such ionization and recombination source terms or parallel temperature gradients are negligible. In this dissertation, 3DLIM is applied to regions of the very far-SOL where collector probes were inserted; a region where a simple SOL prescription is more appropriate. The justification of this assumption is shown in section 3.3.5. In 3DLIM a synthetic collector probe is inserted into a 3D volume, and the plasma solution adjusts to the sink action of the probe. This means flows are imposed between the probe face and the respective target it faces, such that plasma is flowing towards the probe face on the half closest to the probe, and away from the probe on the half closest to the target (refer back to Fig. 2.12). The location of where to inject impurities into the 3DLIM volume is user specifiable. In section 3.3.5 it is shown how the injection location can be scanned to reproduce empirical trends in the deposition patterns, and in chapter 4 we show how DIVIMP can be used to guide 3DLIM input. Once injected, impurities are followed one at a time through successive stages of ionization until deposition on a probe face or one of the absorbing boundaries, thus creating simulated deposition profiles.

### 3.2.3 Python

The programming language of choice for data analysis for this dissertation is Python due its open-source design, widespread use in fusion, and ease of learning. To that end, a GitHub was setup for the fusion group under David Donovan with a number of useful scripts at https://github.com/ORNL-Fusion/utk-fusion. Without going into details, the most useful scripts are outlined in Table 3.1. These scripts were used extensively in the following sections.

### 3.3 Trends and reproductions of experimental measurements

In this section we go over experimental results and trends of collector probes inserted during MRC, as well as reproductions of the results in 3DLIM. In section 3.3.1 we show experimental measurements from RBS and LAMS of tungsten deposition profiles and indicate the key
observations that later are reproduced in 3DLIM. In section 3.3.2 we present an empirically derived scaling law that suggests the power entering the SOL and the connection length are the two most important factors in determining how much W deposited on the CPs. Section 3.3.3 demonstrates how the number of exponential fall off lengths of the plasma density in the SOL may be a more appropriate metric for distance from the separatrix in the context of CPs. Section 3.3.4 presents 3DLIM simulations of deposition patterns and shows that it is most appropriate to treat radial impurity transport in the far-SOL as convective and not diffusive. Section 3.3.5 shows how the observation that W deposition peaked along the edges of the probes is reproduced in 3DLIM only when assuming a simple SOL prescription.

3.3.1 RBS and LAMS measurements of deposition patterns

As shown in Fig. 3.2, RBS and LAMS were used to measure the deposition profiles along the length of the probes. LAMS has the additional capability to measure across the faces to enable measurements of 2D deposition profiles. Fig. 3.5 shows an example 2D profile from one of the 0.5 cm probes. In the contour plot, the left edge corresponds to the tip of the CP, while the top and bottom correspond to the edges (in machine coordinates the up/down direction is the poloidal). The already highlighted trend that more W was collected near the tips is evident here, but an additional unexpected observation was that W deposition peaked on the edges. In the plot on the right of Fig. 3.5 the average poloidal profile obtained by averaging along the radial direction is shown to highlight this edge peaking observation. The observant eye may notice that the poloidal width shown here is only 0.25 cm wide despite the probe being 0.5 cm wide. This is simply due to the machining of the probes where the actual deposition area that is machined flat only takes up 0.25 cm of the probe. Further analysis of these 2D profiles is continued in section 3.3.5.

LAMS is also capable of providing isotopically resolved measurements of the deposition profiles. Fig. 3.6 demonstrates how a 2D deposition profile of the total W deposition can be split into the relative contributions from each isotopically unique W ring. This is done through use of a stable isotopic mixing model (SIMM) [17, 62, 64]. For the probe in this figure we can see that most of the W was sourced from the shelf ring, except that the W
Table 3.1: Table of Python scripts

<table>
<thead>
<tr>
<th>Script</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>get_lp</td>
<td>Access, filter and plot target Langmuir probe data for input into DIVIMP</td>
</tr>
<tr>
<td>oedge_plots</td>
<td>Large collection of plotting and data formatting scripts for analyzing DIVIMP results.</td>
</tr>
<tr>
<td>oedge_plots_gui</td>
<td>GUI interface for oedge_plots for rapid DIVIMP analysis</td>
</tr>
<tr>
<td>get_cp_data</td>
<td>Access collector probe data from MDSplus database and map to plasma coordinates</td>
</tr>
<tr>
<td>lim_plots</td>
<td>3DLIM plotting routines</td>
</tr>
</tbody>
</table>

Figure 3.5: Example 2D profiles measured via LAMS indicating the increased W deposition along the edges of the CPs. The right plot is the average poloidal profile obtained by averaging along the radial direction.
deposited along the edges seemed to have mostly come from the floor ring. This is a curious observation that presents an opportunity for future analysis.

The RBS (and LAMS, not shown) data showed a significant dependence on the connection length for each side, Fig. 3.7. Fig. 3.7a shows plunging Langmuir probe $n_e$ data in black with the OTF and ITF connection lengths in blue. Fig. 3.7b show the ITF and OTF RBS data for the collector probe inserted for this shot with the same connection length data in blue. Note the log y-scale for both these plots. Finally Fig. 3.7c visualizes where each plateau in the ITF connection length data occurs. If we look at the ITF connection length, we can see that most radially furthest out field lines limit on portions of the outer wall, here labelled “Wall”. This corresponds to a connection length of between 0.2-1.0 m. Moving radially inwards more, the connection length abruptly increases at the location indicated by a pink 1. This is where field lines begin to clear the outer wall and begin to limit on portions of the upper baffle. This corresponds to a connection length of about 2-3 m. As we move radially inwards further, the ITF connection length experiences another abrupt increase at the location signified by a pink 2. This is where field lines clear the upper baffle and start to limit on the upper divertor region, where connection lengths are around 10 m. From Fig. 3.7b we can see that this CP, as with all the others, do not go further than field lines limiting on the upper baffle. We can define this region of the baffle-limited SOL out to the wall as the very far-SOL, a term we have been using already in this dissertation. Finally, the dashed blue line is the OTF connection length, which is relatively constant and is around 8 m.

The effect of going from wall to baffle-limited is apparent in both the $n_e$ and ITF data. In the $n_e$ data, the exponential fall off length decreases when going from the baffle to wall-limited region. This is commonly observed in plunging Langmuir data [49]. A similar effect is seen in the ITF data (solid circles in Fig. 3.7b). Such a dramatic effect is not seen in the OTF data (open circles) where the connection length is constant. This suggestion of a strong dependence on the connection length is analyzed from two different angles in this chapter. Section 3.3.2 looks at how changes in the OTF connection length, which was about constant and in the range of 6-8 m for each probe, could explain how much W ultimately deposits on the CP. Section 3.3.4 attempts to explain the observed steepening in the ITF profiles by assuming W radially transports via convection instead of diffusion.
Figure 3.6: Demonstration of the SIMM model in which the relative contributions from each W ring is measured by taking advantage of each ring’s isotopically unique W signature.

Figure 3.7: a) Black circles are the plunging Langmuir probe \( n_e \) data from shots #167192-195. In blue is the connection length data for each direction, either the ITF or OTF. b) RBS data for the ITF (filled circles) and OTF (open circles) sides with the same connection length data in blue. c) 2D cross section showing physically where each plateau in the ITF connection length occurs.
3.3.2 Scaling law of total W deposited on collector probes

A concern for all collector probe experiments is if a statistically significant amount of impurities will be deposited on the probes. For most probes inserted during MRC a significant amount of W was deposited, though not all of them. Thus, it is of first-order importance to figure out what conditions gave the most deposition to understand under what plasma conditions CPs are applicable. In this section we present an empirical scaling law suggesting that the power entering the SOL ($P_{SOL}$) and the connection length ($L_{conn}$) are the most controlling factors.

A scaling law is an empirical relation used to predict or explain a set of experimental measurements. Scaling laws are popular in tokamak physics due to the amount of physical processes that are still not well-understood, i.e. scaling laws can be used to predict outcomes without needing to understand all the underlying physics. They have been used to understand the controlling physics in the heat flux width [38] and the energy confinement time (see chapter 14.5 of [25] for a few other popular examples). The scaling law in Eq. 3.4 consists of fitting the total amount of W per shot deposited on a collector probe to the equation:

$$W_{\text{total}} = a \cdot P_{SOL}^b \cdot L_{conn}^c.$$  

(3.4)

An arbitrary example demonstrating two extremes of a scaling law is shown in Fig. 3.8, where the prediction from the scaling law is plotted on the x-axis and the actual experimental data is on the y-axis. On the left plot is an example of a perfect scaling law, where the result of the fit perfectly reproduces the actual experimental data. In the right plot is a scaling law that does not reproduce the experimental data at all. In more physical terms, for the perfect scaling law one can say that the chosen independent variables likely capture the main controlling physics mechanisms behind the experimental data. Conversely, the imperfect scaling law does not capture the controlling mechanisms. Realistically, decent scaling laws will fall somewhere between these two extremes.

For our experiment, the Python function curve_fit which is part of the scipy library was used to fit the unknown coefficients a, b and c in Eq. 3.4. The choice of the independent
variables $P_{SOL}$ and $L_{conn}$ were decided on through trial and error of testing a combination of various plasma related parameters. Other parameters tested in the scaling law include distance from the separatrix, triangularity, ELM frequency, $q_{95}$ and $\lambda_{ne}$ (see next section). It is noted that a more thorough analysis could use principal component analysis to better decide on the most important physics parameters. The results of fitting the total W deposited to this scaling law is shown in Fig. 3.9. The data is restricted to probes inserted during favorable $B_T$ ($B_x\nabla B_y$) H-mode shots due to the fact most probes were inserted for these conditions, as well as just the OTF sides of the probes since the ITF side $L_{conn}$ could vary by as much as 10x along the length (Fig. 3.7). The OTF sides were relatively constant, falling somewhere in the range of 6-8 m for each probe. This figure suggests that $P_{SOL}$ and $L_{conn}$ may be the primary controlling factors in determining how much W deposits on a collector probe.

The connection length dependence is perhaps not too surprising, as a larger connection length means more plasma volume from which to collect W from for the probe. A parameter scan in 3DLIM was performed on a generic collector probe demonstrating a similar trend, the results of which are shown in Fig. 3.10. In this plot, the radial deposition profiles are plotted for three different simulations where the connection length was set to either 3, 5 or 7 m. It is apparent the lower connection length simulations led to less W collected, as expected, though the trend shown here is not as strong as the scaling law predicts, i.e. decreasing the connection by about a factor of 2 in 3DLIM decreases the amount collected by almost 10x, not $2^{4.5}=23x$.

The $P_{SOL}$ dependence is likely more complicated to quantify, but there are two possible physics mechanisms that $P_{SOL}$ contributes to that could qualitatively explain it. First, a larger $P_{SOL}$ could generally lead to higher target temperatures, which in effect could lead to increased sputtering and thus W in the SOL. Second, the ion temperature gradient force (the FiG in Eq. 2.3) would likely be stronger with increased $P_{SOL}$. The FiG force is directed upstream and would thus encourage “leakage” of impurities out of the divertor region. The sub-field of impurity leakage is an interesting one on its own, but is unfortunately beyond the scope of this dissertation. An area for further analysis would be to compare two probes with identical $L_{conn}$ but different $P_{SOL}$, and then to generate SOL plasma backgrounds with
Figure 3.8: Examples of a perfect scaling law (left), and a horrible one (right).

Figure 3.9: An empirical scaling law where the total amount of W collected by the collector probes is reproduced via a fit to $P_{SOL}$ and $L_{conn}$.
either OSM or SOLPS and inject impurities into them. Two candidates have been identified in Fig. 3.11, designated by their probe names A18 and A23. Both these probes were inserted for favorable $B_T$ H-mode shots and have identical connection lengths of 6.54 m. $P_{SOL}$ was about 3.5x higher for A18 compared to A23, likewise with the total W per shot deposited. This alone provides evidence for the nearly direct scaling of total W per shot with $P_{SOL}$ observed in the scaling law of Fig. 3.9, i.e. a 3.5x increase in $P_{SOL}$ corresponds with about a 3.5x increase in W per shot. Further analysis on this topic would likely be to perform a case study on these two probes.

### 3.3.3 $\lambda_{ne}$ as a metric for distance to separatrix

This section attempts to address the question of how close does the collector probe need to be to the separatrix to sample an accumulation, should it occur? It seems the answer to this question may not be necessarily how far the probe is, but rather how many plasma density exponential fall off lengths, $\lambda_{ne}$, away it is. $\lambda_{ne}$ is obtained by performing an exponential fit to the portion of the Thomson scattering data that extends out into the SOL. An example of this process is shown in Fig. 3.12 where we have plotted $n_e$ against R-Rsep at the OMP. In this example, $\lambda_{ne} = 5.75$ cm. We know that for the probe that was inserted during this shot, the tip was 7.49 cm away from separatrix. Thus this probe was $7.49/5.75 = 1.30 \lambda_{ne}$'s away from the separatrix.

Performing this process for each probe and then plotting the result with the Total ITF/OTF Ratio, which is the ratio between the sum of all the tungsten on each side of a probe, results in Fig. 3.13. There is a trend in this graph that within about 2 $\lambda_{ne}$, the ITF side begins to collect more tungsten than the OTF, though there is likely more to it than that, namely that the only probes with ITF/OTF confidently greater than one were in for unfavorable $B_T$. A truly ideal set of data would have data for say 1-6 $\lambda_{ne}$ for both $B_T$ directions, something that was targeted in the methane experiments of chapter 5.

The conclusion to draw from this section is that, ignoring $B_T$ direction and assuming a near-SOL impurity accumulation does exist, then the collector probe would need to be inserted within at least $2\lambda_{ne}$ from the separatrix. But there seems to be distinguishing characteristics to be made between the magnetic field direction and whether it was in the
Figure 3.10: 3DLIM parameter scan in connection length for an arbitrary collector probe demonstrating the correlation in W deposited and $L_{\text{conn}}$.

Figure 3.11: Two probes inserted during favorable H-mode shots with identical connection lengths. $P_{\text{SOL}}$ and the W deposited per shot both differed by about 3.5x in support of the observed direct scaling with $P_{\text{SOL}}$ from Fig. 3.9.
**Figure 3.12:** Example of fitting an exponential to the plasma density from Thomson scattering to extract the plasma density fall off length, $\lambda_{ne}$.

$$y = 9.57e^{-\frac{x}{5.76}}$$

**Figure 3.13:** The ITF/OTF total tungsten content for each probe plotted against how many $\lambda_{ne}$s it was from the separatrix. Each data point represents a specific probe. The direction of the toroidal magnetic field is distinguished by the colors.
favorable or unfavorable direction. Namely that for the probes within a range of 1-2 $\lambda_{ne}$, unfavorable Bt resulted in much higher ITF deposition. This is something we are building up to in chapter 4 where we discover two of the probes on this graph were inserted a similar number of $\lambda_{ne}$’s from the separatrix but had different $B_T$ directions.

### 3.3.4 Convective vs. diffusive radial transport in reproduction of deposition patterns

Nearly all impurity transport studies, as well as most background SOL plasma codes like OSM and SOLPS, assume radial transport is diffusive. This is treated via a tunable parameter called the “anomalous diffusion coefficient”, $D_{\perp,\text{anom}}$, or just $D_{\perp}$. For instance, in codes like SOLPS it is common to treat $D_{\perp}$ as a radially varying constant that is adjusted such that the resultant radial profiles of $n_e$ and $T_e$ match the respective Thomson scattering profiles (e.g. Fig. 1 and 2 of [46]). In impurity transport codes like DIVIMP, the radial transport coefficients are tweaked to match experimental impurity measurements. In a series of papers on DIVIMP modelling for a set of $^{13}C$ injection experiments during DIII-D, $^{13}C$ deposition profiles along the targets were used as experimental constraints on the impurity modelling [21, 19, 22]. Despite decades of relative success in treating the impurities as radially diffusing, the evidence backing up the diffusive assumption is lacking. Even more, the diffusive theories consistently fall short in predicting the strength of the radial transport in the SOL, see chapter 4 in [53].

Radially convective transport of the plasma is commonly observed on all major tokamaks (and even linear plasma devices). Comprehensive reviews of this intermittent convective, or "blobby" transport is covered in [74, 15]. As early as 2001 it was recognized in DIII-D that about 50% of the radial transport in the SOL was controlled via blobs [9]. Indeed as we will show in this section, 3DLIM simulations required convective radial transport of W instead of diffusive to correctly reproduce collector probe deposition profiles.

In Fig. 3.14 a 2D cross section of the 3D 3DLIM simulation volume is shown. The coordinate system is such that left/right is the parallel along the field line direction, and the up/down is the radial direction. At the left boundary is the outer target, while the right
is actually the upper baffle and outer wall. This is due to the fact collector probes during MRC were rarely, if ever, inserted beyond field lines that were not limited on the upper baffle. This region of the SOL is often called the windowed region, the peripheral plasma, or the very far-SOL. At the radially furthest out points the fields actually begin to limit on portions of the outer wall, which is here represented as a 4x decrease in $L_{\text{conn}}$. The top of the figure represents the simulation boundary towards the main part of the SOL, and the bottom represents the wall. The left, right and bottom boundaries are all absorbing boundaries, while the top is a reflecting boundary (chapter 3.2.2). A synthetic collector probe is shown in this volume and the two designated faces, the ITF and OTF. Also designated is the connection lengths from each probe face to a boundary, demonstrating the significantly higher $L_{\text{conn}}$ for the OTF side. In this volume a 3D plasma solution is generated that takes into account the sink action of the CP faces on the parallel flow. The plasma is a ”simple SOL” prescription (section 3.3.5) due to being in the very-far SOL. At the top of the simulation volume shown in red is the impurity injection region to simulate an impurity source into the very-far SOL from the main SOL. This injection region can cover the entire length of the plasma as shown, or it can be specified to only cover a particular area of the domain.

The results of a scan in the radial diffusion coefficient is shown in Fig. 3.15a and b. These two plots show the deposition profiles plotted against distance from the separatrix for the ITF and OTF sides of a CP on a log y-scale. The dots are from RBS with black dashed lines as exponential fits to the RBS data to guide the eye, while the solid lines are from 3DLIM. The colored lines with error bars are the best fits from 3DLIM using a radial diffusion coefficient of $10 \, m^2/s$. For this particular simulation, an ITF-directed W source was imposed to match the observation of more W on the ITF sides compared to the OTF, and a simple SOL prescription is used. $n_e$ and $T_e$ data from a plunging Langmuir probe were used as input to generate the background (Fig. 3.17). One can see that for the OTF side in purple, $D_\perp = 10 \, m^2/s$ matches the experimental RBS data well. For the ITF side, it also matches up until $R - R_{\text{sep}} = 10$ cm, where the RBS data steeply drops off. This also happens to be the location where the connection length decreases from 2 m to 0.5 m for the ITF side.
Figure 3.14: 2D cross section of a 3D 3DLIM simulation volume.

Figure 3.15: ITF and OTF deposition patterns. Dots are RBS data and dashed black lines are fits to the data to guide the eye. Solid lines are results from a 3DLIM radial diffusion coefficient scan. Colored lines with error bands are the best fit of $10 \text{ m}^2/\text{s}$. 
Figure 3.16: Comparison of diffusive and convective transport in 3DLIM. Convective transport captures the steep drop in the profile due to the decreased connection length.
In Fig. 3.16, comparisons for the ITF side are shown under diffusive transport at 10 \( m^2/s \) and convective transport at 125 m/s. It is apparent that the steep drop off observed in RBS is reproduced under convective transport considerations, but not under diffusive. A possible explanation lies in the fundamental nature of each process. Convective transport is implemented relatively simply in 3DLIM: impurity ions travel radially at a constant velocity of 125 m/s. Diffusive transport is by nature a Monte-Carlo process involving semi-random steps in both radial directions. The random nature may act to flatten out the deposition profiles as diffusion naturally does. Convection lacks this flattening out capability as the ions are radially transporting, in a sense, ballistically. One could imagine the ions as a bullet travelling horizontally (radially) along the surface, where gravity (parallel flows to the probe face) acts to bring the bullet to the surface. As to the value of 125 m/s, it is worth noting that this is around the measured radial velocity of blobs in the very-far SOL of DIII-D [49, 9].

### 3.3.5 Simple SOL prescription in 3DLIM

Up till now 3DLIM simulations have assumed a simple SOL prescription, and whether or not that is appropriate can be estimated from the SOL collisionality. Using Eq. 4.106 from chapter 4 of [53] we can estimate the SOL collisionality in the very-far SOL:

\[
\nu^*_{SOL} \approx 10^{-16} nuL/T_u^2. \tag{3.5}
\]

\( T_u \) and \( n_u \) are the upstream plasma temperature and density, respectively, and \( L \) is the connection length. \( \nu^*_{SOL} \) is unitless. Using plunging Langmuir probe data from a representative L-mode shot, a rough estimate of the collisionality is plotted in Fig. 3.17. The \( T_e \) data has been set to a minimum of 5 eV due to a) unreliability of Langmuir probe data below about a few eV and b) plasma profiles typically flatten out in the far-SOL of L-mode shots due to intermittent or blobby transport [49]. The peaking of \( \nu^*_{SOL} \) around \( R=R_{sep} = 6.5 \) cm is likely not physical, but the purpose of this plot is to just give order of magnitude estimates of \( \nu^*_{SOL} \). Collector probes typically were inserted no further than about \( R=R_{sep} = 7-8 \) cm.
Figure 3.17: Reciprocating $n_e$ and $T_e$ Langmuir probe measurements taken during DIII-D L-mode shots #167192-195 plotted with the estimated SOL collisionality in green.

Figure 3.18: Regions of collisionality for different regimes of the SOL. Figure reproduced from [53].
From [53], it is stated that $\nu^*_\text{SOL} \lesssim 10$ is the simple SOL regime, $10 \lesssim \nu^*_\text{SOL} \lesssim 50$ is a regime of intermediate collisionality between the simple and complex SOL regimes, while $\nu^*_\text{SOL} \gtrsim 50$ is the complex SOL regime. These guidelines are reproduced in Fig. 3.18. At R-Rsep = 8 cm, the tip of most CPs, $\nu^*_\text{SOL} \approx 60$, and then monotonically decreases as we approach the outer wall. This suggests that CPs may exist in a mixed regime of simple and complex SOL, but as we will show later in this section, 3DLIM simulations suggest a simple SOL prescription may be most appropriate in regards to matching CP deposition profiles. Furthermore, in H-mode the inter-ELM $n_e$ and $T_e$ profiles are typically lower compared to L-mode data shown here (again, see [49]), thus making the simple SOL prescription even more likely in H-mode.

As presented in Fig. 3.5, 2D deposition profiles showed increased W deposition along the edges of the probes. To reproduce similar trends in 3DLIM, a simple SOL prescription was required. In Fig. 3.19a the average poloidal profiles (i.e. the deposition profiles averaged along the radial direction) from a set of 3DLIM simulations are shown [72]. In these simulations, an impurity source in only the ITF direction is imposed. The solid lines are using a simple SOL, while the dashed lines are a complex SOL. It is shown that the peaking along the edges is reproduced only in the simple SOL, and only on the OTF side (the side opposite the impurity source). No peaking is observed on either of the ITF profiles.

A proposed explanation for edge peaking is as follows. Poloidal peaking is an inherently 3D effect. Consider a W ion following a parallel field line towards the ITF face. Assume the field line, and thus the ion as it travels along it, narrowly passes by the ITF face. At this point the OTF face is in the W ion’s “rearview mirror”. Further assume that the W ion poloidally diffuses onto a field line that connects back to the OTF face. The background plasma flow is then towards the OTF face, and in the absence of thermal forces (negligible $T_{e,i}$ gradients in the simple SOL), the net force on the W ion will then be towards the OTF face due to the friction force, thus turning the W ion around to deposit on the OTF face. How far across the OTF face the W ion will travel poloidally before depositing is determined by the parallel flow speed and $D_{\text{poloidal}}$, and since parallel speeds are much higher than cross-field speeds, the W ions tend not to deposit very far from the edges, resulting in an increase in W content there. Thus, peaking along the poloidal edges of a probe face is a result of...
W initially coming from the opposite direction. A possible reason this is not observed in a
complex SOL in 3DLIM is due to the fact that the net force on the W ions towards CP faces
is weaker due to the $T_e,i$ gradient force away from the faces. Thus, the net force required
to turn the W ions around is either significantly diminished or practically non-existent. A
rather simplified “flipbook” style of images to demonstrate this process is shown in Fig. 3.20.

Fig. 3.19b demonstrates a parameter scan in $D_{poloidal}$ from 1.0 to 0.02 m$^2$/s to attempt
and reproduce the severity of peaking. While the relative location of the peaking is
reproduced, the severity is under represented, likely pointing out the deficiencies in our
basic implementation of the parallel flows. To quantify the severity of the peaking we can
take the ratio of the edge value to the center value. The left edge had a normalized value
of about 0.9 W deposition, while the right had about 0.83. Meanwhile the center was about
0.53. The average ratio between the sides and the center is $(0.90/0.58 + 0.83/0.58) / 2 =
1.49$, i.e. there was about 1.5x more W on the edges compared to the center of the probe.

Doing this for each side of a probe and dividing the OTF peaking by the ITF gives the
OTF/ITF Peaking ratio. A ratio greater than 1 indicates more peaking on the OTF side,
and a ratio less than 1 means more peaking on the ITF side.

Fig 3.21 demonstrates the relationship between the ratios of the total amount of W
deposited versus the relative severity of the peaking on each side. The ITF/OTF Total W ratio is simply the total W deposited on the ITF side divided by the total amount on
the OTF side. Thus Fig. 3.21 tells us that generally more W deposited on the ITF sides
generally means larger peaking on the OTF side, and vice-versa. Physically, ITF/OTF Total
$> 1$ indicates W enters the far-SOL from the ITF side, i.e. above the CP when
inserted in DIII-D. As discussed in the previous paragraph, the peaking along the edges is a
result of W arriving from the opposite direction, and thus ITF/OTF Total should directly
correlate with OTF/ITF Peaking; OTF/ITF Peaking is a secondary indicator of the primary
direction of the W source into the far-SOL. To support these statements, 3DLIM simulations
were performed where the impurity source was moved from completely OTF-directed to
completely ITF-directed, blue stars in Fig. 3.21. The lowest left star is a completely OTF
source, while as one moves towards the top right the source moves towards a completely
ITF source. The simulation results track experimental results rather well, suggesting the
Figure 3.19: a) Average poloidal deposition profiles from 3DLIM comparing the two types of SOL prescriptions. b) Comparison of a parameter scan in the poloidal diffusion coefficient to experimental LAMS measurements.

Figure 3.20: Series of flipbook style images to help explain the reason behind peaking on the edges of CPs.
Figure 3.21: Ratio of the total amount of W collected on each probe side plotted against the ratio of the severity of the edge peaking. Circles with error bars are experimental measurements separated by $B_T$ direction, and blue stars are from 3DLIM.
admittedly rudimentary plasma implementation in 3DLIM contains much of the controlling physics of deposition profiles.

### 3.4 Summary of experimental MRC collector probe trends

This chapter introduced the hardware and software used in this dissertation as well as reviewed the primary trends and experimental measurements from collector probes inserted during MRC. A scaling law was derived that implied $L_{\text{conn}}$ and $P_{\text{SOL}}$ are the two most important factors in determining how much W deposits on CPs. This analysis in particular offered a viable area for future research in simulating the effect the $P_{\text{SOL}}$ may have on total W deposition. We then showed how the ITF/OTF Total W ratio increases above 1 when the tip of the CPs are within $\sim 2 \lambda_{\text{ne}}$’s from the separatrix, though the role of the $B_T$ direction was unable to be separated in this trend. Chapter 4 attempts to elucidate these $B_T$ dependent effects. We then showed how interpretive modelling of the CP deposition patterns with 3DLIM suggests radial impurity transport in the very far-SOL is best modelled using convective instead of diffusive considerations. This was required to reproduce the effect that a changing $L_{\text{conn}}$ had on the steepening of the deposition profiles. Finally, we showed that in order to reproduce the peaking in deposition along the edges of the CPs required a simple SOL prescription in 3DLIM. The relative amount of peaking between the two CP sides trended $\sim$linearly with the ITF/OTF Total ratio, suggesting that the peaking measurements can be considered a secondary indicator of the primary entrance location of W into the very far-SOL.
Chapter 4

The effect of parallel flows on hypothesized near-SOL impurity accumulation

4.1 Introduction

One of the largest issues facing current and future tokamaks is core contamination by impurities. This includes helium from the D-T reaction, impurity gases injected for power dissipation, such as Ne, as well as impurities sputtered by plasma material interactions (PMI). The latter follow the “impurity chain”: sourcing from the targets and walls, transport through the scrape off layer (SOL), and ultimately core contamination. Sourcing of impurities is relatively well-understood with widely available databases of sputtering yields [5] and reliable diagnostics capable of monitoring the ionization rate of sputtered neutrals [1]. Core contamination is relatively well studied and understood as well, since it has long been known that a fusion reactor will only be able to reach ignition with a core tungsten (W) concentration of less than 10-5 [45]. The transport of impurities through the SOL is the least understood part of the impurity chain and is crucial in determining the level of core contamination as the impurity density along the separatrix between the X-points sets the boundary condition on core impurity content. This lack of understanding
is primarily due to the fact that the SOL is an under-diagnosed region of the plasma. Recent studies have nevertheless made significant advances in understanding edge impurity transport despite the lack of direct measurements of impurity ion density along the separatrix between the X-points. Indirect evidence has been obtained, in SOLPS modelling comparing the magnitude of leakage between different injected impurities on ASDEX-U [52], also in DIVIMP simulations of the expected W distributions in preparation for the DIII-D Metal Rings Campaign [20], as well as EDGE2D-EIRENE/DIVIMP code comparison studies of radial W profiles on JET [35].

SOL impurity transport involves both parallel-to-B and radial transport. Radial transport is typically modelled assuming either an anomalous diffusion coefficient or a radial convective velocity, or some combination of the two. In a fluid treatment, impurity ion parallel transport is due to the five major forces in Eq. 2.3 (repeated here for convenience):

\[
F_Z = -\frac{1}{n_Z} \frac{dp_Z}{ds} + m_Z \frac{v_i - v_Z}{\tau_s} + Z e E + \alpha_e \frac{d(kT_e)}{ds} + \beta_i \frac{d(kT_i)}{ds} + \ldots \tag{4.1}
\]

Equation 4.1 neglects the inertial force (the ma side of \( F = ma \)). Neglecting this term is an appropriate approximation for low-Z impurities [52], but for heavier impurities like W this approximation may be less accurate [55].

Simulations have shown that the FiG and FF usually dominate [52]. The FiG is largely responsible for the long-hypothesized near-SOL impurity accumulation [42]. This force is directed up the temperature gradient, i.e. away from the targets, due to the higher collision frequency between impurity ions and lower temperature background ions, \( (1/\tau_{iz}) \sim T_i^{-3/2} \). Therefore, the FiG directs impurities in the near-SOL (where Ti gradients are strong) to a region along the field line where Ti peaks, e.g. near the outer midplane, OMP, or the crown of the plasma, leading to accumulation of impurities. This is an undesirable effect as it creates a region of elevated impurity density at the separatrix, the boundary of the confined plasma.

The FF is the force exerted on impurity ions due to collisions with plasma background (fuel) ions. Mach probes inserted into single-null, attached, L-mode discharges generally
indicate a strong toroidal field (BT) dependence on parallel flow in tokamak SOLs: JT-60 [34], DIII-D [7], Alcator C-Mod [36], ASDEX-U [41] and JET [23]. As summarized in [6], for the B_T direction unfavorable for H-mode access (ion Bx∇B drift away from X-point), fuel parallel flows stagnate about halfway between the targets and flow away from the stagnation region towards each target. For the opposite B_T direction, fuel parallel flows stagnate somewhere between the OMP and the X-point with relatively fast (M∼0.3-0.5) inner-target directed, ITD, flows throughout most of the SOL. The origin of these flows is still under investigation, but they are evidently a combination of a number of effects: intrinsic edge momentum [7], Pfirsch-Schluter flows [12], ExB return flows [12] and ionization-driven flow reversal [8]. While 2D fluid codes such as EDGE2D and SOLPS have qualitatively reproduced these flow patterns, they tend to report lower velocities than are experimentally measured [12] and thus may under-represent the effect of the FF on SOL impurity transport. It is thus crucial that modelling of impurity transport in the SOL include the effect of B_T dependent parallel flows. In this study, additional flows are therefore imposed ad hoc to simulate the experimental situation.

DIII-D is a graphite armored device with one of the most comprehensively diagnosed SOLs in present tokamaks, making it an excellent facility to study the transport of W as a trace particle. To this end, DIII-D executed the Metal Rings Campaign (MRC) where two rings of toroidally symmetric, isotopically different W tiles were installed in the lower, outer divertor, figure 1 [31]. Double-sided graphite collector probes (CPs) were inserted at the OMP on the MiMES reciprocating drive [16][71] where they remained for a set number of discharges. To avoid re-erosion of deposits on the CPs, they were inserted no deeper than 7 cm from the separatrix and were connected along field lines that limited on protruding regions of the vessel wall, placing them in what is defined as the “wall-SOL” [49], see Fig. 1. The CPs were removed between discharges and subsequently analyzed with Rutherford backscattering (RBS) at Sandia National Laboratory (e.g. see [66]), and with laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS, or LAMS) at Oak Ridge National Laboratory [17], to measure the W deposition profiles both along (radially) and across (poloidally) the faces of the CPs. LAMS can distinguish individual W isotopes as well. The experimental layout is shown in Fig. 4.1. The lowest W ring (the “floor” ring)
consisted of natural W (26.5\% \textsuperscript{182}W); the higher ring (“shelf” ring) consisted of isotopically enriched W (93\% \textsuperscript{182}W). Using the LAMS data and a stable isotope mixing model (SIMM) \cite{17}, the fractional contribution from each W ring to the total W measured on each CP could be measured. In Fig. 4.1 the CP is shown at the OMP, where each side of the CP is designated as either the inner target facing (ITF) or outer target facing (OTF) side. Also shown is the location of Langmuir probes installed along the outer target, as well as both Thomson scattering arrays. In Fig. 4.1, the SOL is subdivided into three distinct regions: the near-SOL (purple), the far-SOL (orange) and the wall-SOL (tan). These definitions are adhered to throughout this paper.

The MRC consisted of \(\sim 500\) discharges covering a wide variety of conditions: L-mode/H-mode, low/high power, lower single/double null configurations and for both \(B_T\) directions. A total of 57 CPs were inserted over the course of the campaign. This chapter reports a case study of two probes inserted into similar H-mode discharges that primarily differed in the \(B_T\) direction. The organization of the chapter is as follows. Section 4.2 compares the two discharges, indicating their similarities and differences. In section 4.3, the 1D fluid solver OSM-EIRENE \cite{54} is used to generate background (fuel) plasma solutions for each discharge that are constrained using experimental target Langmuir probe and upstream Thomson scattering data. Using DIVIMP \cite{58}, W ions are injected into these backgrounds to obtain predicted poloidal distributions of impurities near the separatrix. OSM-EIRENE generates parallel flow patterns that are qualitatively similar to those expected during (L-mode) unfavorable \(B_T\) operation. To represent the expected favorable \(B_T\) flow patterns, a scan of \textit{ad hoc} imposed ITD flows was used. Localized near-SOL accumulation of W ions, clearly separate from near target \(n_z\) peaks, is observed for the unfavorable \(B_T\) case. For no imposed flows, localized near-SOL accumulation is also observed for the favorable \(B_T\) case, but with applied flows of \(M \geq 0.3\) the accumulation is mostly “flushed out”. This demonstrates the significant effect that fast parallel flows can have on W distributions in the near-SOL. Section 4.4 shows how each case informs input specifications to the Monte Carlo impurity transport code 3DLIM which is used to model the wall-SOL in order to interpretively model each CP deposition pattern. To successfully reproduce the deposition patterns in 3DLIM for unfavorable \(B_T\), it is found that the far-SOL W source feeding into
Figure 4.1: Poloidal cross-section of DIII-D showing the location of both W rings and the collector probe and its two sides. Also shown are the target Langmuir probes, and Thomson scattering measurement locations. Pertinent locations of the vessel are indicated: the upper divertor, the upper baffle and the outer wall. The SOL regions are qualitatively subdivided into the near-SOL (purple), far-SOL (orange) and wall-SOL (tan).
the wall-SOL must be strongly skewed in the ITF direction, consistent with the occurrence of near-SOL impurity accumulation found in the DIVIMP modeling of the near-SOL. For favorable $B_T$, 3DLIM found that the far-SOL W source feeding into the wall-SOL is unskewed towards either the ITF or OTF side of the CP, consistent with the DIVIMP finding of little/no near-SOL accumulation for $M \geq 0.3$ applied flows. Finally, section 4.5 discusses implications of these results regarding SOL impurity transport simulations before concluding remarks.

4.2 Experimental setup: similar shots differing primarily in $B_T$ direction

During the MRC CPs were inserted into two similar NBI-heated H-mode discharges differing primarily in the $B_T$ direction. Time traces comparing the two discharges are shown in Fig. 4.2. Fig. 4.2(a) shows the equal but opposite $B_T$ fields; the salmon line, #167247, is for the favorable $B_T$ configuration; the purple line, #167277, is for the unfavorable $B_T$ configuration. Fig. 4.2(b) compares the line-averaged densities. Each discharge operated at similar densities close to $5 \times 10^{19} \text{ m}^{-3}$, but the unfavorable $B_T$ discharge experienced an instability at $\sim 4200$ ms. Fig. 4.2(c) compares the power entering the SOL, $P_{\text{SOL}}$, calculated by subtracting the core radiated power from the total injected power. For the favorable $B_T$ discharge, $P_{\text{SOL}} \sim 1$ MW, slightly higher than the unfavorable $B_T$ discharge ($\sim 33\%$ higher). Fig. 4.2(d) compares time traces of the outer strike point location, with the range of the W metal ring on the floor indicated in purple. The favorable $B_T$ strike point was positioned slightly inboard of the W ring. Fig. 4.2(e) compares the ELM characteristics of each discharge, showing the slightly higher ELM frequency of the unfavorable $B_T$ discharge. The Greenwald fractions for the unfavorable and favorable $B_T$ discharges were similar, 0.75 and 0.82, respectively. Both discharges operated with plasma currents of 1.3 MA and a $q_{95}$ of 4.0.

Although not identical, these discharges are sufficiently similar to make meaningful comparisons of the CP depositions patterns when the only major change is the $B_T$ direction. The most significant discrepancy may be the difference in strike point location. This likely modifies the source rate of W from the floor ring due to the peak heat flux being slightly
Figure 4.2: Time traces of some key parameters comparing similarities and differences between two DIII-D discharges.
displaced from the ring in the favorable $B_T$ discharge; however, this is allowed for by injecting ions into the simulation volume from the X-point, section 4.3. This approximation assumes that the W leaks out of the divertor region and reaches the X-point, which is confirmed by the significant amounts of W measured on each CP. This prevents quantitatively estimating the absolute W densities in the SOL, but it will be shown that this does not prevent identification of the controlling physics governing the transport of W in the near- and wall-SOL. Differences in ELM frequency also modify the source rates of the W rings [63]; injecting W ions at the X-point in the simulations addresses this as well. Differences in $P_{\text{SOL}}$ and density are allowed for by modelling each discharge separately.

Fig. 4.3 shows the connection lengths for each side of the CP plotted against distance from the separatrix at the OMP. The far-SOL and wall-SOL regions are colored orange and tan, respectively (see Fig. 4.1). The connection lengths for each CP side are nearly identical for each discharge. The OTF sides of the probe are characterized by a roughly constant connection length of $\sim 7$ m along flux tubes extending down to the outer target. The ITF sides are more complicated, as the connection length varied significantly with distance from the separatrix. For $R - R_{\text{sep}} = 6.0$ to $7.5$ cm, if the CP had been inserted this far, the ITF sides limited on portions of the upper divertor/inner wall (see Fig. 4.1). For $R - R_{\text{sep}} = 7.5$ to 10 cm, the ITF sides limited on the upper baffle. Beyond 10 cm, the field lines limited on the outer wall. The entire region from the upper baffle outwards defines the wall-SOL. In section 4.4 it will be shown that the CP deposition patterns are very sensitive to abrupt changes in the connection length, and therefore it is essential to account for them.

It is instructive to highlight one additional point in contrasting the two discharges under consideration. Each discharge had similar $\lambda_{ne}$'s: 3.33 cm for the unfavorable discharge, and 3.08 cm for the favorable discharge. This corresponded to each probe being inserted 1.5 and 2.1 $\lambda_{ne}$'s from the separatrix for the unfavorable and favorable $B_T$ discharges, respectively. It is noted that the contrasting ITF/OTF ratios of the collector probes, which will be shown later, are not easily explained by the trend of Fig. 3.13 in section 3.3.3. I.e., despite being a similar number of $\lambda_{ne}$'s from the separatrix, the ITF/OTF ratios differed by about a factor of 5. This observation is in fact what led to the analysis of this chapter, in particular asking the question of if there were any $B_T$-dependent effects that should be considered.
Figure 4.3: Connection lengths for each side of a CP inserted at the midplane for DIII-D discharge #167247 (unfavorable B_T, solid lines) and #167277 (favorable B_T, dashed lines). The surface each field line limits on is indicated for each face. The far-SOL and wall-SOL are colored orange and tan, respectively (see Fig. 4.1).
4.3 Interpretive modelling with OSM and DIVIMP

To simulate SOL W impurity transport in each of these discharges the OEDGE suite of codes is used. The 1D fluid equation solver OSM (Onion Skin Model) coupled with the Monte-Carlo neutral code EIRENE is used to generate $n_e$, $T_e$, $T_i$ and $v_i$ profiles along each individual flux tube, thus creating a plasma background for each discharge. The kinetic Monte Carlo trace impurity transport code DIVIMP is then used to inject W ions into the plasma background to generate 2D W distributions. A scan in ad hoc imposed ITD fuel parallel flows is carried out in DIVIMP to assess the effect fast parallel flows have on the W spatial distributions in the near-SOL.

4.3.1 OSM: empirical reconstruction of the background plasmas

OSM-EIRENE (OSM: onion-skin modeling; EIRENE: Monte Carlo neutral hydrogen code) is an interpretive code that solves the 1D fluid equations (see chapter 9 of [53]) along individual flux tubes using a Runge-Kutta solver. As much experimental data as possible is input to OSM to empirically reconstruct the background plasma. The solver splits each flux tube at a specified midpoint and solves each half of the flux tube separately “from each target up”. Experimental target $n_e$ and $T_e$ data, primarily from embedded Langmuir probes, is provided as input and is used to self-consistently solve for $n_e$, $T_e$, $T_i$ and $v_i$ along each half-tube. The solver is iterated with EIRENE to provide particle, momentum, and energy source terms to each respective 1D fluid equation. To constrain the upstream profiles, the OSM profiles are compared to experimental Thomson scattering $n_e$ and $T_e$ measurements for each flux tube. Several additional options are often required to achieve sufficient agreement with upstream Thomson scattering measurements such as per-tube modifications of near-target momentum loss or minor modification of the input target data (the probe and Divertor Thomson data are typically not in exact agreement). The OSM version used here does not explicitly include ExB drifts, although they are implicitly included by virtue of using target $n_e$ and $T_e$ data as input, i.e. the experimental target data by definition includes all physics effects. Uncertainties in the background reconstruction are primarily for regions without experimental data to constrain the OSM model. Once the data is sufficiently constrained,
a smoothing algorithm is applied to force the solution for each half-tube to match at their junction.

For the following reconstructions, the inter-ELM experimental data are used to generate background plasmas. OSM reconstructions of the background plasma for the unfavorable B_T discharge are shown in Fig. 4.4. Fig. 4.4(a) and (b) give the target Langmuir probe T_e and saturation current (j_sat) profiles. Also included are the respective measurements of the lowest divertor Thomson scattering (DTS) chord, which is ~5 mm above the target surface. Typically, the outer strike point is swept to “fill in” the target Langmuir probe profiles for each flux tube (i.e. each \( \psi_N \)), but for the discharges considered in this study the strike points were stationary and thus target data are only available at the discrete Langmuir probe locations. To provide continuous and smooth input to OSM, the target profile fitting method often used for parallel heat flux profiles [18] is adapted here for T_e and j_sat profiles: an exponential convoluted with a Gaussian is fit to each respective peak, while the regions outside the peak are fit to an exponential. Fig. 4.4(a) and (b) demonstrate that this method adequately captures the characteristics of the peaks near the strike point. The input T_e data in Fig. 4.4(a) away from the peak are between the Langmuir probe and DTS measurements. Such disagreement between the Langmuir probe and DTS data is not uncommon, and it is necessary to make a choice of which to use. Fitting an input profile that passes between both the measurements resulted in reasonable agreement with the upstream Thomson scattering measurements, Fig. 4.4(c) and (d). Fig. 4.4(c) and (d) show radial profiles of T_e and n_e for OSM and the Thomson scattering measurements mapped to the OMP, demonstrating that the OSM solution is mostly constrained by the Thomson scattering data. The largest disagreement is in the n_e data beyond ~2 cm from the separatrix, where the OSM density is roughly 2x higher than Thomson scattering measurements. The reason for this is seen in the comparisons of the OSM solution to Thomson scattering data along the flux tubes, Fig. 4.4(e) and (f). Fig. 4.4(e) shows that the parallel OSM T_e data fall well within the error bars of the experimental Thomson scattering T_e data from the core and divertor systems, but Fig. 4.4(f) shows that the density data do not fall within error bars. OSM was unable to generate parallel density profiles that simultaneously matched both divertor and core measurements, so the choice was made to generate solutions.
that passed between the DTS and core Thomson measurements. This explains why the OSM density of Fig. 4.4(d) was generally slightly higher than the experimental core TS data. A possible reason for not simultaneously matching core and divertor Thomson data is uncertainties in mapping the R, Z location of each Thomson measurement to the plasma equilibrium. The inner target half of the flux-tubes used outer target Langmuir probe data to construct a solution since comprehensive inner target data were unavailable for this discharge. This introduces ambiguity to the results close to the inner target, although even if inner target Langmuir probe data were used, strong volumetric losses likely occur there that the OSM model currently does not consider, which would make the results ambiguous in any case. These considerations mean that OSM/DIVIMP results near the inner target are only considered approximate.

The same comparisons between OSM and experimental data for the favorable B_T discharge are shown in Fig. 4.5. In Fig. 4.5(a), reasonable agreement with upstream Thomson scattering T_e data was obtained by preferentially matching the input data to the Langmuir probes. The radial OSM density profiles match the core Thomson scattering data much better for this discharge. The increased peaking of the density data very near the targets in Fig. 4.5(f) compared to Fig. 4.4(f) is due to the addition of momentum loss along this flux tube, which in OSM acts to push the density peak away from the target and to increase the density in a flux tube. Outer target data was again used for the inner target.

As discussed in section 4.1, experiments in L-mode plasmas have shown substantially different flow patterns for each B_T direction. While the pair of discharges under consideration are H-mode, they may still be compared to the expected L-mode flow patterns under the assumption that the experimentally measured flow patterns are at least roughly independent of operating mode. While this assumption lacks supporting Mach probe data, it is noted that the physics behind the hypothesized effects that contribute to each flow pattern (Pfirsch-Schluter flows, ExB return flows, etc.) are not limited to L-mode. It is also noted that radial transport may be significantly different in H-mode than L-mode, which could modify parallel flow patterns. Fig. 4.6 compares the OSM parallel flows in flux tubes 3.71 cm from the separatrix at the OMP, placing it just outside the near-SOL. The flow pattern in
Figure 4.4: OSM comparisons to experimental data for discharge #167247 (unfavorable $B_T$). a, b) OSM input compared to target Langmuir probe data. c, d) Upstream comparisons of OSM solution to experimental Thomson scattering data. e, f) Along-tube comparisons of OSM solutions with Thomson scattering data from the “core” and DTS systems.

Figure 4.5: Similar comparisons for discharge #167277 (favorable $B_T$).
unfavorable $B_T$ is qualitatively similar to that expected from experimentally measured L-mode flow patterns, specifically that flow stagnates about halfway between the targets and then flows towards each respective target. The favorable $B_T$ flow pattern (solid line) shows a similar flow pattern, but as discussed in section 4.1, fast inner target flows of order $M = 0.3-0.5$ are expected in favorable $B_T$ (L-mode) discharges. The dashed line is the OSM flow with a conservative *ad hoc* addition of $M = 0.3$ ITD flows. As will be shown in the next section, a conservative estimate of $M = 0.3$ is sufficient to largely prevent localized near-SOL W accumulation.

4.3.2 DIVIMP: injection of impurities and the effect of fast parallel flows in the near-SOL

As discussed in section 4.1, SOL impurity transport simulations have long-predicted near-SOL impurity accumulation due to the FiG. Here it is proposed that near-SOL W accumulation tends to only occur for the unfavorable $B_T$ direction, while for favorable $B_T$ the expected fast ITD flows tend to mostly “flush out” accumulation.

DIVIMP is provided a plasma background, such as that generated by OSM, and it follows individual impurities in a Monte Carlo way to generate impurity distribution statistics. One can launch impurities from the targets to simulate physical sputtering or inject impurities at any specified location in the plasma. Initial DIVIMP simulations using the plasma backgrounds of section 4.3 launched W ions from the two metal rings, but effectively no W was able to leak out of the divertor region, a prediction known to be incorrect since W was measured on all CPs. This indicates two potential inadequacies in these OSM+DIVIMP solutions, a) modeling of near-target conditions and/or b) modeling the launch of W ions. It appears likely that both factors contribute to the erroneous DIVIMP prediction of divertor leakage, as DTS data near the floor ring were unavailable to constrain the OSM background near the target. The sheath physics and prompt redeposition models in DIVIMP are also only approximate. In addition, DIVIMP did not model the arcing that was experimentally observed on the shelf ring [11] which could cause non-negligible amounts of W to sputter with appreciable energies (penetration mean free paths). Further, W transport due to ExB
Figure 4.6: OSM results for parallel flows of the fuel plasma for a flux tube 3.71 cm from the separatrix for each simulated background (fuel) plasma. Also shown is the parallel flow for a favorable \(B_T\) case with additional \(M = 0.3\) ITD background plasma flows imposed \(ad\ hoc\).
drifts was not included, which have been shown to have a significant effect on W leakage and transport below the X-point [43]. The focus of the present study, however, is not on divertor leakage but on transport of W above the X-points with regard to near-SOL accumulation; therefore, the issue of leakage has been circumvented by injecting W ions at the X-point in DIVIMP and considering only normalized impurity density.

Fig. 4.7 shows DIVIMP results for the normalized W density along a near-SOL flux tube plotted against distance from the inner target for the flux tube 9 mm from the OMP-separatrix for various scenarios. The injection location of the W ions (near the X-point) is shown by a dashed line. A radial diffusion coefficient $D_\perp = 0.3 \text{ m}^2/\text{s}$ was specified for the W ions. Dots along each curve indicate where the parallel W velocity goes to zero (impurity stagnation point, ISP). The case representative of discharge #167247 (unfavorable $B_T$) is shown in bright purple, where background plasma flows stagnate (fuel stagnation point, FSP) about halfway between the targets with flow towards each target otherwise, as in the example shown in Fig. 4.6. Localized near-SOL W accumulation is evident by the large peak in W density at about 45 m from the inner target. In black is the W density for the case representative of discharge #167277 (favorable $B_T$). Localized near-SOL accumulation occurs for this case as well, but this DIVIMP case lacks the ITD flows that are often observed in (L-mode) favorable $B_T$. A scan of imposed ITD flows from $M = 0.1$ to 0.5 was carried out, the results of which are shown as the rest of the colored lines of Fig. 4.7. As can be seen, the additional flows a) shift the near-SOL accumulation towards the inner target b) shift the ISP towards the inner target c) decrease the magnitude of accumulation, and d) increase the width of the accumulation region. Indication of localized near-SOL accumulation largely disappears with imposed flows of $M = 0.3$, which is on the lower end of the range of experimentally measured flows of $M = 0.3-0.5$. The relative magnitude of accumulation is estimated by the ratio between the peak impurity density and the background impurity density (for the favorable $B_T$ simulations in Fig. 4.7 the background can be considered the low point at $\sim 50$ m from the inner target, normalized density $\sim 0.1$ for each case). Thus, the magnitude of accumulation decreases from $\sim 10x$ the background level for $M = 0$ to $\sim 3x$ the background for $M = 0.3$ to 0.5, a significant reduction. The highest density value for each
case occurs either at or near the ISP, as expected, though this demonstrates the existence of an ISP does not ensure that localized accumulation will occur.

The existence of impurity accumulation does not depend on just the parallel forces on the impurity ions, but also on the radial particle exhaust rate (i.e. anomalous radial diffusion) to the far-SOL. If the radial exhaust rate is strong enough, impurities may be removed faster than they can accumulate, which in principle could cause a local impurity density rarefaction, rather than a peak. Fig. 4.8 shows a scan of the radial diffusion coefficient, $D_\perp$, for the unfavorable $B_T$ simulation. Up to about $D_\perp=0.4 \text{ m}^2/\text{s}$ evidence of substantial, localized near-SOL accumulation at the ISP is apparent, but past 0.6 m$^2$/s the increased radial diffusive exhaust rate near the ISP prevents accumulation from occurring. In fact, the profiles show density rarefaction instead of accumulation above 0.6 m$^2$/s. As discussed in [55], this implies that at heightened levels of radial diffusion, acceleration-rarefaction in the parallel impurity flux is likely occurring near the ISP. Increasing the radial diffusion coefficient has no effect on the location of the ISP, as intuitively expected. Increased radial plasma transport near the separatrix is already attractive from a heat-flux perspective as it is thought to increase the parallel heat flux width [70], and this demonstrates it may also be attractive from the impurity transport perspective as it lowers the near-SOL impurity density and can prevent accumulation for a given impurity source strength.

4.3.3 Characterizing the far-SOL W source feeding into the wall-SOL

The far-SOL impurity distribution at the interface between the far-SOL and the wall-SOL is the impurity source feeding W ions into the wall-SOL. The DIVIMP computational grid stops before reaching the wall-SOL, thus there is a radial gap between the far-SOL distribution of W at the outer edge of the DIVIMP grid and the location where the actual wall-SOL source is located. While the W distribution at the outer edge of the DIVIMP grid is not precisely the W source feeding the wall-SOL, it should be indicative of the actual situation since the dominant parallel forces are not expected to differ significantly between far-SOL and wall-SOL.
Figure 4.7: DIVIMP results for total W density profiles along a flux tube 9 mm from the separatrix for varying levels of imposed Mach number. Dots along each curve indicate where the parallel W velocity goes to zero (impurity stagnation point, ISP).
**Figure 4.8:** DIVIMP results of a scan in the W radial diffusion coefficient for a near-SOL flux tube 2.7 mm from the separatrix. Dots along each curve indicate where the parallel W velocity goes to zero (ISP).
Shown in Fig. 4.9 is the W distribution in the far-SOL flux tube at the outer edge of the DIVIMP computational grid (6.7 cm from the OMP-separatrix) for each simulated discharge. The region along the flux tube that covers the same poloidal range as the wall-SOL is shaded. The simulated distribution in the region near the wall-SOL for the unfavorable B\textsubscript{T} discharge is characterized by being largely skewed towards the inner target direction. Conversely, for the favorable B\textsubscript{T} simulation, the distribution near the wall-SOL is relatively flat (the slight skewing towards the outer target direction is a code artifact due to placing the W injection location near the X-point). These DIVIMP far-SOL W distributions may be used to guide the specification of the W source distribution that feeds into the wall-SOL, a region the 3DLIM code is designed to simulate in order to interpretively model CP deposition patterns.

4.4 3DLIM simulations

3DLIM [59][72] is a 3D Monte Carlo impurity transport code designed to simulate impurity transport in the wall-SOL where the CPs are located. A 2D cross section of the simulation region for the unfavorable B\textsubscript{T} case is shown in Fig. 4.10. The coordinates are radial (R), parallel-to-B (B) and poloidal (P, into the page). The OTF side of the region is on the right, while the ITF side is on the left. The bottom represents the outer wall, and the top represents the interface between the far-SOL and wall-SOL, where a W source distribution is specified. Absorbing boundaries are imposed at the outer target, outer wall and upper baffle, and reflecting boundaries are imposed at the far-SOL/wall-SOL interface as well as the poloidal bounds. The connection length from the OTF side to the outer target is approximated as a constant 7 m, while the ITF side is divided into two regions to approximate limiting on either the upper baffle or portions of the outer wall. Constant connections lengths of 2 and 0.5 m are set for these regions, respectively (see Fig. 4.3). This simulation region spans R-R\textsubscript{sep} = 7-15 cm. 3DLIM follows impurity ions one at a time until deposition on either an absorbing boundary or a CP face.

Ideally, the DIVIMP computational grid would extend to the far-SOL/wall-SOL interface, and the parallel W density profiles at the interface would be directly imported into 3DLIM, effectively coupling the two codes. 3DLIM would convert the parallel density distribution to
Figure 4.9: W density profiles for a far-SOL flux tube at the outer edge of the DIVIMP computational grid. The region at the same poloidal location of the entrance to the wall-SOL is shaded. The unfavorable $B_T$ simulation is characteristic of a far-SOL distribution of W in the wall-SOL region skewed in the inner target direction. Conversely, the favorable $B_T$ distribution is relatively flat.
Figure 4.10: 2D cross-section of the 3D 3DLIM simulation region for the unfavorable $B_T$ case. The distance from the OTF face to the outer target is approximated as a constant 7 m. The ITF side is split into two regions: upper baffle-limited and outer wall-limited, each with approximate connection lengths of 2 and 0.5 m, respectively. A W source feeding ions from the far-SOL into the wall-SOL is specified at the top of the simulation region in red. Shown above is the parallel W distribution at the edge of the DIVIMP grid near the far-SOL/wall-SOL interface (dashed) and the interpretively chosen W distribution at the far-SOL/wall-SOL interface in 3DLIM.
a probability distribution, from which the initial location of W ions into the 3DLIM region is chosen from. Unfortunately, limitations in grid-making software make it very difficult to generate computational grids that radially extend up to the far-SOL/wall-SOL interface. In this study, the edge of the DIVIMP computational grid is \( \sim1-2 \) cm away from the far-SOL/wall-SOL interface, thus the parallel W density distributions, such as those in Fig. 4.9, cannot be directly imported into 3DLIM. Therefore, the initial W location probability distribution must be treated as an interpretive input to the model (i.e. the probability distribution is a "knob" to turn in 3DLIM input). Although, the general characteristics of the DIVIMP parallel distribution of W density may be used to help guide 3DLIM input, such as if the parallel distribution should be skewed towards the inner or outer target.

The normalized parallel W distribution from the edge of the DIVIMP computational grid for the unfavorable \( B_T \) discharge is shown at the top of Fig. 4.10 (dashed line). This distribution is the same that is shown in the shaded region of Fig. 4.9; it is the source at the edge of the grid near the far-SOL/wall-SOL interface, but not at the interface. The observation that the distribution is skewed towards the inner target direction is used to generate a 3DLIM probability distribution from an exponential (solid line). The interpretive modelling of this section determined an exponential characterized by a 1/e decay length of 0.65 m best reproduced experimental CP deposition patterns. This distribution is notably more skewed in the ITF direction compared to the DIVIMP distribution at the edge of the computational grid. This may be due to differences in connection lengths; the parallel W distribution from DIVIMP is along a field line \( \sim50 \) m long, while the far-SOL/wall-SOL interface in 3DLIM is only \( \sim9 \) m long. Experimentally, the background plasma is sensitive to changes in connection lengths (consider the changes at the far-SOL/wall-SOL interface in the experimental radial profiles of \( n_e \) and \( T_e \) in [49]), therefore the difference between the DIVIMP and 3DLIM W distributions may be due to differences in the background plasma. Addressing this issue would require a DIVIMP computational grid that extends to the far-SOL/wall-SOL interface.

The simulation region for the favorable \( B_T \) direction is similar to Fig. 4.10, except the probe tip was inserted radially \( \sim1 \) cm past the upper baffle flux-surface, i.e. slightly past the far-SOL/wall-SOL interface. The field lines beyond the far-SOL/wall-SOL interface limited
on portions of the upper divertor/inner wall (refer to Fig. 4.3), and thus experimentally the ITF side is divided into upper divertor, upper baffle and outer wall-limited regions. Due to code limitations in 3DLIM, the ITF side of the simulation region is only split up into two regions: an upper divertor-limited region that is 7 m away from the ITF face, and an upper baffle-limited region that is 2 m from the ITF face. This corresponds to $R-R_{\text{sep}} = 6$-15 cm. Since the tip of this probe is now closer to the edge of the DIVIMP computational grid, the favorable $B_T$ source in Fig. 4.9 is more representative of the appropriate source distribution feeding into the 3DLIM region. Indeed, the interpretive modelling of this section determined a W source distribution not skewed in either direction to be most appropriate, quite similar to Fig. 4.9.

### 4.4.1 Background plasma prescription

The background plasma in 3DLIM is chosen to be either a completely convection or conduction-limited SOL [53], as it presently lacks the more sophisticated 1D fluid equation solver in OSM-ERIENE. It was shown in [72] that a convection-limited SOL prescription in the wall-SOL was appropriate for an L-Mode discharge of similar geometry based on estimates of collisionality using data from a plunging Langmuir probe. Additionally, experimentally observed patterns in the CP deposition profiles were only reproduced with a convection-limited SOL prescription. Plunging Langmuir probe data are not available for the two discharges under consideration in this paper and thus collisionality estimates are unavailable. There were no measurements of $n_e$ and $T_e$ in the wall-SOL of these discharges, but constant values of $n_e$ and $T_e$ of $1 \times 10^{18}$ m$^{-3}$ and 2 eV, respectively, were estimated and used. These low wall-SOL densities and temperatures are characteristic of H-mode discharges in DIII-D [49].

A fuel stagnation point (FSP) in the background plasma velocity in 3DLIM is imposed halfway between each target, with flow speeds linearly increasing to the sound speed in approaching each target. The perturbing effect of inserting a probe into the simulation volume is accounted for by treating each probe face as a target, creating a FSP between it and each target it faces in the flux tubes subtended by the probe and plasma flows toward
the probe faces. The effect of ELMs on the background plasma and impurity transport is not included.

4.4.2 Reproduction of deposition profiles and ITF/OTF ratio

3DLIM launches impurity ions with a specified (parallel) probability distribution and follows them until deposition on an absorbing boundary (i.e. the wall structure) or CP face. Radial transport is outwards towards the outer wall and can be treated as diffusive or convective, or some combination of the two. Simulations in [72] found that best agreement with measured deposition profiles was with a purely convective prescription. This was due to the interplay between impurity radial transit time and changes in parallel velocity with a changing connection length such as that on the ITF side in Fig. 4.10.

Fig. 4.11 compares 3DLIM results with experimental RBS and LAMS measurements for the ITF and OTF sides of each probe. All data have been normalized to facilitate comparison (note log scale). The left column of plots are the two sides of the probe inserted for unfavorable B_T while the right column is for favorable B_T. The top (bottom) row is the ITF (OTF) sides. The ITF sides are designated by which vessel surface the field lines were limiting on, either upper divertor limited (UDL), upper baffle limited (UBL) or outer wall limited (OWL). For each probe, this corresponds to connection lengths of \( \sim 7, 2 \) and 0.5 m. The field lines connecting to the OTF sides connected to the vessel floor and were approximately constant at 7 m. The effect of a changing connection length is most evident in the ITF side of the probe inserted for unfavorable B_T when transitioning from the UBL to the OWL region, corresponding to a \( \sim 4x \) decrease in connection length. The exponential decay of the deposition profile steepens in the OWL region for the experimental RBS and LAMS data as well as the simulated 3DLIM data. This probe was inserted up to the far-SOL/wall-SOL interface, thus experimental data in the UDL region are unavailable for this probe. Data for the OTF side of this probe are also well-reproduced in 3DLIM.

For the probe inserted for favorable B_T, no steepening in the deposition profiles when transitioning from UBL to OWL is observed, though LAMS data do show slight changes in the profiles near the transition. It is not clear why the probe inserted for favorable B_T does not respond as strongly to the UBL to OWL transition. 3DLIM results do not reproduce the
steepening in profiles because the decrease in connection length was not implemented at this location. This probe was inserted ~1 cm further into the plasma than the probe inserted for unfavorable B_T, providing a single RBS data point in the UDL region. LAMS data are not available due to a destructive chemically based ICP-MS method that had been used in this region before LAMS measurements were made. 3DLIM reproduces the RBS observation that the deposition profiles flatten off in the UDL region. In 3DLIM, this is due to a longer connection length. Data for the OTF side are relatively well-reproduced except for R-R_{sep} >12 cm. The LAMS and RBS data show a slight steepening in the OTF deposition profile. This may be due to approaching the detection limit of RBS and LAMS.

These simulations modeled W ions assuming purely convective radial transport at constant speeds of 275 and 225 m/s for the unfavorable and favorable B_T direction, respectively. As discussed in [72], the radial convective speed in 3DLIM required to reproduce deposition patterns is close to measured radial blob speeds in DIII-D, suggesting interaction between W ions and blobby transport; qualifying this hypothesis will require further study. The W radial velocity in the unfavorable B_T simulation was 50 m/s higher than in favorable B_T, suggesting slightly enhanced radial transport in the unfavorable B_T direction; more definitive conclusions will require wall-SOL measurements of n_e and T_e. The sound speed, and thus background plasma flow in 3DLIM, depend on T_e, and on how far W ions radially transport before deposition; the latter is inversely proportional to the strength of the parallel flow as a stronger parallel flow acts to force impurities towards a target in a shorter radial distance.

The most informative measurement the CPs make is the deposition ratio between the two sides, the ITF/OTF ratio. This measurement quantifies the asymmetry between the two faces and provides a representation of the primary impurity flux direction toward the probe. ITF/OTF >1 indicates the majority of impurity flux is arriving from the ITF direction, and vice-versa. The ITF/OTF ratio along each probe plotted against distance from the separatrix is shown in Fig. 4.12. LAMS data are shown as the error banded line, while 3DLIM results are the bold lines. The CP inserted for unfavorable B_T collected over twice as much W on the ITF side compared to the OTF in the UBL region. The probe inserted for favorable B_T collected more W on the OTF side along the entire length of the probe.
Figure 4.11: 3DLIM reproductions of experimental RBS and LAMS data for both the ITF and OTF sides of each CP. The ITF sides are divided into regions designated by the vessel surface that field lines limited on: Upper divertor limited (UDL), upper baffle limited (UBL) and outer wall limited (OWL). Field lines connected to the OTF sides were approximately of constant length about 7 m.
Even for the tip of the CP which extends in past the far-SOL/wall-SOL interface (the UDL region), 3DLIM predicts the ratio remains at or below 1.

In 3DLIM, ITF/OTF <1 in the UBL region is observed in the favorable B_T simulation despite using an unskewed far-SOL W source feeding into the wall-SOL, i.e. a flat W distribution at the far-SOL/wall-SOL interface. The OTF side is characterized by a region ∼7 m long, while the ITF side is only ∼2 m long, i.e. the OTF region is 3.5x larger than the ITF region. Therefore, the OTF side of the CPs in UBL region sample a much larger plasma region, which with a flat W distribution results in the OTF side collecting more W, driving the ITF/OTF ratio below 1. Thus, it is surprising that in the unfavorable B_T simulation and the corresponding measured deposition patterns, ITF/OTF >1 was ever observed; despite the ITF region being 3.5x smaller than the OTF region, the ITF side of the CP collected over twice as much W. This indicates that the conclusion that W enters the wall-SOL from the ITF direction is a robust one.

In summary, ITF/OTF >1 indicates that W entered the wall-SOL from the ITF direction, which DIVIMP simulations in fact found in the spatial distribution near the far-SOL/wall-SOL interface during strong localized near-SOL W accumulation (unfavorable B_T). These results demonstrate that the CPs have provided the first indirect evidence of near-SOL W accumulation – and for the unfavorable B_T direction only. For the favorable B_T direction, near-SOL W accumulation was not indicated by the CP deposition patterns, evidently due to fast inner-target flows flushing out most of the W ions that would otherwise accumulate.

4.5 Conclusions

This chapter presents simulations for two similar H-mode discharges differing primarily in the B_T direction. OSM was used to generate plasma backgrounds for each discharge using respective target Langmuir probe data and constraining the solutions with upstream Thomson scattering data. DIVIMP was then used to launch W ions near the X-point separatrix, finding the formation of localized near-SOL W accumulation roughly midway between X-points. It was next shown in the favorable B_T DIVIMP simulation, that imposed ad hoc inner target directed flows with M ∼ 0.3 largely prevented near-SOL accumulation by
flushing out W ions that otherwise would accumulate, indicating that accumulation tends to occur for unfavorable B_T only. Next, the far-SOL W distributions from DIVIMP were used to specify the far-SOL W source feeding into the wall-SOL used in 3DLIM. 3DLIM then successfully reproduced the deposition patterns measured on each CP. To reproduce the unfavorable B_T deposition patterns, a W source skewed in the ITF direction was required, consistent with the spatial distribution of W near the far-SOL/wall-SOL interface in the corresponding DIVIMP simulation. For the favorable B_T direction, an unskewed source, i.e. favoring neither the ITF or OTF direction, was required to reproduce measured deposition patterns, again consistent with results from the DIVIMP simulation with an imposed inner-target-directed flow of M = 0.3. In summary, by reproducing the most important features of the CP deposition patterns, OSM+DIVIMP+3DLIM simulations demonstrate that localized near-SOL W accumulation occurs for the unfavorable B_T direction only, while for favorable B_T fast inner-target flows largely flush out accumulation.

Several assumptions were made in this study. A major assumption is that flow patterns characteristic of L-mode plasma also existed in the simulated H-mode discharges used in this paper. The effect of ELMs was also neglected. The OSM-ERIENE solutions close to the inner target are only rough estimates owing to lack of experimental data to constrain the model as well as neglect of volumetric power and pressure losses. For the DIVIMP simulations used to specify the 3DLIM input, a radial W diffusion coefficient of 0.3 m^2/s was imposed in the entire DIVIMP computational grid; however, doubling the coefficient can prevent localized near-SOL accumulation from occurring. In 3DLIM a convection-dominated background prescription was assumed, and radial impurity transport was treated as purely convective. Furthermore, the effect of re-erosion of deposited W on the CPs is neglected in 3DLIM. Each of these assumptions indicate areas for improvement of in this type of study. An improvement in future work will be to directly import the far-SOL impurity distributions calculated by DIVIMP into 3DLIM, i.e. directly coupling the two codes; this will require that the DIVIMP computational grid be extended to the far-SOL/wall-SOL interface. Importing the actual connection lengths, as in Fig. 4.3, instead of approximating the ITF region as two regions with constant connection lengths, will also improve the fidelity of the 3DLIM results.
The findings reported here demonstrate the need to take into account the $B_T$ dependent flow patterns of the background plasma when modelling SOL impurity transport in the tokamak boundary. It has been shown that using a conservative estimate of expected plasma flows for favorable $B_T$ can have a first-order effect on the spatial distribution of W in the SOL. The lack of any localized near-SOL W accumulation for favorable $B_T$ does not necessarily imply lower core concentrations, as the issue of W leakage from the divertor was circumvented in these simulations by injecting W ions at the X-point. It is possible that for favorable $B_T$ large enough divertor leakage could outweigh the advantage of weak/no near-SOL impurity accumulation. To study these effects, an inclusive study of leakage and global SOL impurity transport is needed, requiring more diagnostic coverage than was available in this study.
Figure 4.12: 3DLIM reproductions of the ITF/OTF ratio along each probe along with experimental LAMS data.
Chapter 5

Isotopic methane injection experiment

The results of the collector probe experiments during MRC motivated the execution of another dedicated collector probe experiment. This chapter outlines the motivation and preparation that went into the collector probe methane injection experiment that was performed in early 2021. Section 5.1 describes the motivation behind another collector probe experiment and the reasons for some key changes from the MRC experiments. Section 5.2 details the preparation that went into the methane injection experiment, including preliminary modelling and designing a new collector probe. Section 5.3 presents preliminary results and analysis of the experiment. Finally, section 5.4 outlines the need to organize the data from the methane experiment into a standalone database before suggesting topics for future research.

5.1 Motivation

This section outlines the deficiencies of MRC (with regards to collector probe interpretation) and considers the changes and additional diagnostics that were required for the next collector probe experiment. Each decision and diagnostic requirement is discussed one a time to demonstrate the gradual progress towards the methane injection experiment.

The successive collector probe experiment identified the DiMES port as a location to insert an additional collector probe in addition to the one already inserted on MiMES. This requires operating in an upper single null (USN) configuration, Fig. 5.1, such that
both probes are inserted into the main-SOL, defined as the region above the X-point. The probe labeled CP1 is at the previously used location of the collector probes from MRC, and the probe labeled CP2 is at the proposed new collector probe location. The modelling and analysis in chapter 3 demonstrated that peaking along the edges of the probes contained valuable information about the primary impurity flux direction. Therefore, the new collector probes were designed with as wide a collection face as possible. Pictures of new designs with wider collection faces are shown in Fig. 5.1.

The analysis of chapter 4 demonstrated that whether or not localized near-SOL impurity accumulation occurs likely depends on the background plasma parallel flow pattern. Unfortunately, Mach probe measurements were unavailable during the MRC. Therefore, the successive collector probe experiment designated reciprocating Mach probes (RCPs) as a crucial diagnostic. The Mach probe data are taken at the same poloidal location as the collector probes and enables measurement of $n_e$, $T_e$, $v_i$ and Mach numbers. These measurements are very useful in constraining DIVIMP and 3DLIM modelling. A reciprocating probe can be installed on MiMES (MRCP), though this shares the same drive as CP1 so only one may be installed for each discharge (see discussion in later sections on diagnostic vs. collection shots). A reciprocating probe can also be used on the X-point drive (XRCP), which utilizes a separate drive at the same poloidal but different toroidal location as DiMES, therefore XRCP data can be available on every shot. Since parallel flows depend on the $B_T$ direction, the successive experiment executed pairs of similar discharges with opposing $B_T$ direction (the similar discharges used in chapter 4 were for the most part a lucky coincidence that were found by searching the database of MRC shots).

The W rings of MRC were only installed during the summer of 2016, and thus a new method of sourcing trace impurities into the SOL was needed for the next collector probe experiments. Methane injection via the DIII-D gas injection system has a long history of successful applications on DIII-D \cite{2, 57}, yet the carbon in natural methane is 99% $^{12}\text{C}$. DIII-D is a graphite walled device, and thus $^{12}\text{C}$ is far from being as effective a tracer impurity as W was during MRC ($^{12}\text{C}$ is in fact the most abundant impurity atom in DIII-D); it would be impossible to distinguish injected $^{12}\text{C}$ from the $^{12}\text{C}$ sourced from the vessel walls on the collector probe deposition profiles. The other stable carbon isotope, $^{13}\text{C}$ may be considered
Figure 5.1: DIII-D shot #184535. Newly designed collector probes are shown. For reference, the old CP1 design from MRC is shown in the red box. CP1 and the MiMES reciprocating probe (MRCP) share the same drive, and thus are mutually exclusive. CP2 and the X-point reciprocating probe (XRCP) are separated toroidally, and are not mutually exclusive. Colored lines are MDS view chords. $^{13}$CD$_4$ is injected via the upper outer baffle (UOB) injection system, located in the red circled region.
a tracer impurity, as natural carbon is only about 1% $^{13}$C. Therefore, isotopically enriched (deuterated) methane, $^{13}$CD$_4$, can be used to inject $^{13}$C as a trace impurity. Isotopic methane is readily available, and can be attached to one of the gas injection systems on DIII-D. To simulate impurity sourcing from the divertor region, the upper outer baffle (UOB) injection system is the natural choice for USN configurations (see red circled region in Fig. 5.1). The injection location of $^{13}$CD$_4$ via UOB is indicated in Fig. 5.1. Collector probes are machined from graphite, thus to distinguish deposited carbon from the carbon of the probe, the successive collector probe experiment coated the collector probes in silicon to create a carbon-free deposition surface. To measure the $^{13}$C deposition, nuclear reaction analysis (NRA) [65] and LAMS were used since they are capable of distinguishing individual carbon isotopes.

Many higher charge state W lines are in the ultraviolet range (10-400 nm), which made spectroscopic observation of it in the main-SOL difficult during MRC. For instance, the multichord divertor spectroscopy (MDS) system on DIII-D [10] is capable of providing reliable measurements only in the range of about 400-700 nm. The CIII line at 464.7 nm is regularly monitored by MDS, thus carbon is much easier to monitor with MDS than W is. The MDS view chords are shown by the colored lines in Fig. 5.1. The measurements are line-integrated intensities of line radiation, and together can be used to give a general sense of the poloidal distribution of a particular carbon charge state in the SOL. If an accumulation were to occur, then it would appear as a poloidally localized concentration of carbon. The charge exchange spectroscopy (CER) system on DIII-D [13] also regularly uses carbon line radiation to make measurements on parameters such as the plasma ion temperature and toroidal flow in the core and edge. In summary, injecting isotopic carbon into DIII-D enables more efficient use of the existing spectroscopic systems compared to W, strengthening the argument for $^{13}$C as a trace impurity.

This set of motivations are ultimately what motivated the methane injection collector probe experiment. The primary goal is to obtain direct spectroscopic measurements of near-SOL carbon accumulation for the first time. Collector probes inserted on DiMES and MiMES provide secondary supporting measurements. Interpretive modelling using codes
such as DIVIMP, SOLPS-ITER and 3DLIM will be utilized to interpret the experimental results.

5.2 Preparation

In preparation for the methane experiment, a number of tasks were performed ahead of time. Modelling was performed to determine which charge state of carbon is most likely to accumulate so that spectroscopy could be set to monitor the correct lines. A collector probe had never been inserted with DiMES, thus a new probe was designed and tested. A unique plasma shape was also developed, one that had stable strike point control while simultaneously extending far enough down such that the DiMES probe intersected flux tubes sufficiently close to the separatrix. Furthermore, the UOB gas injection system was tested and calibrated for methane.

A set of DIVIMP simulations were performed in a highly-diagnosed L-mode discharge (#167196) with a hypothetical methane puff imposed at the outer strike point, Fig. 5.2. It was shown that the most likely carbon charge state to accumulate was CV, since the temperatures in the accumulation region are too high for lower carbon charge states. Unfortunately, CV lines in the MDS range of applicability are scarce. In the NIST database [44], a CV line at 494.5 nm is theorized to exist, so it was decided to attempt to monitor this line with MDS. Later sections show this line may not have been detected on MDS.

A new collector probe needed to be designed to be inserted on the DiMES. As already mentioned, as wide a collection area is preferable to attempt to capture the edge related effects studied in chapter 3. An image of the newly designed probe is shown as CP2 in Fig. 5.1. A design review was carried out for the DiMES probe to ensure it would survive the expected heat fluxes and possible forces in the event of a disruption [48]. The MiMES collector probe (CP1) was also redesigned with a wider collection area, but the design was sufficiently similar to the previous design that it did not require a dedicated design review. Both collector probes were coated in silicon so that the deposited carbon could be distinguished from the graphite of the collector probe.
Figure 5.2: Hypothetical comparison of CIII and CV distributions with a methane puff at the outer strike point for shot #167196. Simulations and figures courtesy of J. Nichols.
One of the largest preparation tasks was developing a plasma shape that a) had the outer strike point near the UOB plenum b) stable strike point location c) extended close enough to the DiMES probe and d) at least some field lines that connected the MiMES collector probe to the DiMES probe. An ideal time to test plasma shaping is during DIII-D startup, which is an operational window in which DIII-D tests all its systems after a vent in preparation for the next experimental campaign. Multiple startup shots were allotted to develop the required plasma shape. In an effort to bring the plasma towards DiMES, a rigid downwards shift in the entire plasma was performed, Fig. 5.3 left. This resulted in long strike point legs, which are more difficult to control than shorter legs. Instead, elongating the plasma enabled maintaining shorter strike point legs while simultaneously bringing the separatrix close to the DiMES probe, Fig. 5.3 right. It can be seen that relatively far-SOL flux tubes are able to avoid limiting on the vessel floor, enabling the capability of inserting DiMES and MiMES on the same flux tubes. Further iterations on the shaping involved slightly more shaping near DiMES and reducing the flux expansion near the entrance to the outer divertor. The final shape is that in Fig. 5.1 (#184535).

A final preparation task was ensuring correct operation of the UOB gas injection system. During the plasma shaping startup shots, the UOB system injected natural methane into the plasma with the intent of testing spectroscopic detection. Monitoring CIII and CV lines with MDS and CER, it was ultimately determined methane was not being injected as there was no increase in the signals with the methane puff. This ended up being the result of a number of issues. A search in the experimental logbook of DIII-D was carried out with the keywords “UOB” and “leak”, and it was found that there was a number of mentions of a possible leak in the UOB system. Coordinating with the scientists in charge of the gas injection systems confirmed that there was indeed a leak which was subsequently repaired. Furthermore, the valve was found to “stick” shut, meaning it would not open up without a sufficiently high voltage signal. The solution was devised that in the beginning of the voltage programming a voltage spike be included to force the valve open before continuing with the planned voltage programming. Finally, a calibration between the UOB valve voltage and the respective amount of methane flowing out in Torr/L-s was performed. While these fixes
Figure 5.3: Left: USN plasma that has been rigidly shifted downwards towards DiMES, resulting in long legs. Right: USN plasma that has been elongated downwards towards DiMES, resulting in shorter legs and less far-SOL field lines that limit on portion of the floor.
and the calibration were necessary to ensure correct operation of the UOB system, the next section shows the injected methane was still largely undetected.

5.3 Execution and preliminary analysis

The methane experiment was performed as two half-days of experiments in early 2021. The first half-day was in the favorable $B_T$ configuration, while the other half-day was in the unfavorable $B_T$ configuration. The shot plan was to perform a number of “diagnostic” discharges with associated repeat discharges called “collection” shots. Diagnostic discharges operated with the MRCP installed on MiMES, while collection discharges operated with CP1 installed on MiMES (and DiMES). In the diagnostic discharges the strike point was swept to see what strike point location resulted in the most leakage of carbon from the upper divertor (monitored via MDS and CER). The XRCP was installed on all discharges. Table 5.1 contains a summary of the most successful discharges.

Each paired set of diagnostic and collection shots targeted the same plasma density, though difficulty in preventing the density from rising during the course of some discharges meant this was not always the case. The cryopumps were turned off for this experiment to prevent immediate venting of the injected methane, which likely resulted in the walls absorbing significant amounts of deuterium (“wall loading”), meaning the walls were outgassing deuterium during each discharges and increasing the plasma density above the target density. During the course of the experiment it was determined that performing occasional high-powered “cleanup shots” could heat the walls to decrease the wall deuterium inventory and thus improve density control. Time traces of some key plasma parameters for a pair of favorable $B_T$ discharges are shown in Fig. 5.4. #184267 is a diagnostic discharge (red) and #184271 is a collection discharge (purple). The parameters are a) line-averaged density, b) UOB valve voltage, c) injected power, d) the pressure reading near the UOB, e) the strike point location and f) the intensity of an upper viewing filterscope chord monitoring $D_\alpha$ line radiation. The target plasma density was set to $2 \times 10^{19}$ m$^{-3}$, which is maintained for each shot until slightly after the UOB valve opens. The UOB pressure signal confirms that the UOB valve is operating correctly as the pressure increases with each puff, therefore
the increase in density may be from injected methane, but there is not enough evidence to confirm that the injected methane is not only changing the divertor plasma conditions (which the edge density is linked to) without actually leaking out of the divertor region. For example, the methane puff could partially detach the outer strike point without actually leaving the outer divertor, which would modify upstream plasma parameters like the line-averaged density. This topic is currently under investigation. The diagnostic shot strike point sweeps are shown in e). The diagnostic shots performed two sweeps, one before and one during the the methane puff.

While the rise in line-average density is an encouraging sign that methane could be making it into the plasma, a more informative signal would be from one of the spectroscopic diagnostics monitoring carbon, either MDS or CER. In Fig. 5.5 the MDS CIV signal for viewing chord “U5” (green 5 in Fig. 5.1) is shown in blue plotted with the UOB valve voltage for shot #184267. This chord is directed at the outer strike point, and it is expected that it would trend closely with the UOB puff if carbon was actually being injected, but no statistically significant trend is seen. A very slight increase in the MDS may be seen, but this is likely caused by the corresponding slight increase in the line-averaged plasma density. It is expected that the MDS signal would show a more significant increase if carbon was actually leaving the divertor region. For discharges were MDS was set to monitor the 494.5 nm CV line (the charge state most likely to accumulate, Fig. 5.2), there was no reliable indicator that the CV line was being detected. This could be due to either no methane escaping out of the divertor, or that the 494.5 nm CV line is too weak to be detected by MDS.

Data from five different CER chords for discharge #184271 are shown in Fig. 5.6. The chords are labeled according to their “normalized radius” ($\rho$, where $\rho = 0$ is the center of the core and $\rho = 1$ is the separatrix). CER was set to monitor CVI. A rough estimate of the concentration of CVI ($f_C$) at each measurement location can be obtained by dividing the CVI density by the line-averaged plasma density, Fig. 5.6a). $f_C$ starts to increase nearly 1000 ms after the start of the methane puff, suggesting the increased concentration of carbon in the plasma could be due to more than just the density increase (refer back to the discussion of Fig. 5.5), and could be due to injected carbon actually entering the core. This then implies a $\sim$1000 ms delay from puff start to detection in the main plasma, likely due to the time it
Table 5.1: Summary of successful discharges from the methane injection experiments.

<table>
<thead>
<tr>
<th>Direction</th>
<th>Diagnostic Discharge</th>
<th>Collection Discharges</th>
</tr>
</thead>
<tbody>
<tr>
<td>Favorable</td>
<td>#184182</td>
<td>#184183-184</td>
</tr>
<tr>
<td>Favorable</td>
<td>#184267</td>
<td>#184271-272</td>
</tr>
<tr>
<td>Unfavorable</td>
<td>#184527</td>
<td>#184535-536</td>
</tr>
</tbody>
</table>

Figure 5.4: Comparison of a favorable $B_T$ diagnostic (#184267, red) discharge with a collection discharge (#184271, purple). a) Line-average plasma density, b) UOB valve voltage, c) injected power, d) UOB pressure, e) outer strike point location, f) upper viewing filterscope Do intensity.
takes carbon to travel though the SOL. In Fig. 5.6b) the time derivative of $f_C$ is shown. This plot shows acceleration of $f_C$ for each chord starting about 500 ms after the puff, supporting the hypothesis that $^{13}C$ left the divertor region and did not just change the divertor plasma conditions. Qualifying these assumptions that carbon actually escaped the divertor and did not only modify the divertor plasma (in turn modifying core plasma density) is an area of future analysis that may require dedicated modelling, as the entire picture as to where the injected carbon went is still not clear.

NRA and LAMS can distinguish $^{13}C$ from $^{12}C$, and thus can determine if any of the injected carbon transported through the SOL and deposited on the collector probes. Since natural carbon is 1% $^{13}C$, the total measured $^{13}C$ must have the background contribution, i.e. that can be explained by the amount of natural $^{13}C$ already in DIII-D, subtracted from it to yield the “excess $^{13}C$”. In other words, the excess $^{13}C$ is that which cannot be explained by the natural carbon already in DIII-D, and thus must have come from the injected isotopic methane. In equation form,

$$^{13}C_{\text{excess}} = ^{13}C_{\text{total}} - \frac{0.01}{0.99} (^{12}C_{\text{total}}) \quad (5.1)$$

If a statistically significant amount of $^{13}C_{\text{excess}}$ is detected, then it can be assumed some amount of injected carbon escaped the divertor and deposited on the collector probe. The best proof that injected carbon deposited on CP1 is shown Fig. 5.7. This plot shows the centerline profiles of $^{13}C$ as measured by NRA, as well as the excess $^{13}C$ calculated via Eq. 5.1, for a MiMES collector probe inserted during the unfavorable $B_T$ shot #184535. Up to about 40 mm from the tip of the probe statistically significant amounts of excess $^{13}C$ are measured, though beyond this the data is too noisy (negative values indicate noise levels).

Comparison to LAMS data for the same probe is shown in Fig. 5.8. The $^{13}C_{\text{excess}}$ data is in arbitrary units. Similar to NRA, LAMS shows statistically significant amount of $^{13}C_{\text{excess}}$ beyond about 30 mm, though the shape of the deposition profile is different from the NRA profile; the NRA profile shows a gradual increase in $^{13}C_{\text{excess}}$ towards the tip of the probe while LAMS shows a flatter $^{13}C_{\text{excess}}$ deposition profile near the tip with a steeper drop off. The discrepancy between these two methods is a crucial area for further research, as
Figure 5.5: CIV MDS signal for unfavorable $B_T$ shot #184267 (blue) plotted with the UOB valve voltage (green). This signal is for MDS chord “U5” (green 5 in Fig. 5.1). Figure courtesy of J. Nichols.

Figure 5.6: a) CVI density divided by the line-averaged density ($f_C$) for five different CER chords, each at a different normalized radius ($\rho$, center of core is $\rho=0$ and separatrix is $\rho=1$) for shot #184271. b) Time derivatives of each smoothed signal from a). Dashed lines indicate the start of the methane puff (about 2200 ms).
confidence in the shape of the measured deposition profiles is necessary to interpretatively model the profiles in 3DLIM.

The motivation for performing discharges in each B_T direction was to observe the fast inner target flows discussed in chapter 4 such that the effects of the flows on SOL impurity transport can be correctly accounted for in impurity transport modelling. Fig. 5.9 shows the average Mach number for every Langmuir probe plunge taken during the methane experiments. The left plot is for all the XRCP plunges, and the right plot is for all MRCP plunges. The data points are color-coded according to the B_T direction, unfavorable (purple) and favorable (red). See Fig. 5.1 for each measurement location. Positive Mach number indicates flow towards the inner target, while negative is towards the outer target. The data is plotted against the Greenwald fraction \( f_g = \bar{n}_e/10^{20}I_p/\pi a^2 \), \( \bar{n}_e \) is the line-average density in m\(^{-3}\), \( I_p \) is plasma current in A, \( a \) is the plasma minor radius in m).

The expected fast inner-target flows in favorable B_T were observed on the XRCP, with flows of about M = 0.25-0.60. Conversely, for unfavorable B_T, flows in the crown measured by the XRCP were relatively stagnant, generally going no lower than M = -0.2, as expected. The MRCP Mach numbers show no clear distinction between either B_T direction, and varied in the range of about M = -0.4-0.4. It was expected to see the MRCP Mach number correlate with the Greenwald fraction [36], but no such correlation has been observed yet.

The Mach probes also provide radial profiles of \( n_e \) and \( T_e \), which are extremely valuable when it comes to constraining simulated plasma backgrounds. Examples of \( n_e \) and \( T_e \) profiles from two separate plunges during discharge #184267 are shown in Fig. 5.10. The data are plotted against the normalized radius, \( \rho \). Beyond roughly \( \rho = 1.08 \) the data is considered lost in the noise, as evident by unrealistic negative densities (the data are derived from Langmuir probe current-voltage traces, which can report erroneous results if the signal is too low [50]). A total of 101 Mach probe plunges occurred over the course of the experiments, providing a wealth of data that will take time to analyze.
Figure 5.7: Centerline NRA measurements of $^{13}$C and excess $^{13}$C for a MiMES probe inserted during the unfavorable $B_T$ shot #184535. Negative values are due to noise below the detection threshold.

Figure 5.8: Centerline LAMS measurements of the excess $^{13}$C for the MiMES collector probe inserted for the unfavorable $B_T$ shot #184535. Data is in arbitrary LAMS units.
Figure 5.9: Average Mach number for every reciprocating Langmuir probe plunge during the methane experiments plotted against the respective Greenwald fraction. XRCP data is on the left, and MRCP data is on the right. Purple is for unfavorable $B_T$ and red is for favorable $B_T$.

Figure 5.10: Radial profiles of $T_e$ (left) and $n_e$ (right) from two plunges taken during discharge #184267.
5.4 Direction of future analysis

The methane experiments provided a significant amount of data that will require months, perhaps years, to fully analyze and to assemble a cohesive story of impurity transport. The preliminary analysis of these experiments in fact motivated an additional set of methane injection shots that at the time of this writing are still under development. The analysis of these experiments will be a significant undertaking, and will provide data for at least one PhD dissertation, possibly multiple. This section outlines potential areas for future research and the possible results one would hope to obtain from them.

A practical, logistical starting point would be the development of a methane experiment database (MED) filled with information pertaining to these experiments. Many of the plasma parameters (such as injected power, line-averaged density, etc.) are stored on the DIII-D MDSplus database, so there is no need to include those in the MED. The MED should organize the collector probe NRA and LAMS data (both centerline and 2D LAMS deposition profiles) in a consistent format to facilitate analysis and data gathering. The MED should also pair collector probes with respective MRCP and XRCP data (from respective collection and diagnostic shots), which are currently stored in a series of csv files. Valuable connection length data (like that in Fig. 3.17) should also be included in the MED. Furthermore, the measurement locations along the probes should be mapped to machine (R, Z) and plasma (R-R_{sep} and ψ_N) coordinates (see App. A) and stored in the MED to prevent wasted time repeatedly performing such a tedious process. Assembling a MED is crucial to expediting analysis and coordination in an experiment with numerous contributors such as the methane experiments.

Significant effort will be needed to generate background plasma prescriptions for DIVIMP. The increased volumetric losses and possible detachment in the closed upper divertor may require a 2D code such a SOLPS-ITER to generate background prescriptions as OSM-EIRENE is not fully-equipped to handle large volumetric losses or detachment. The plasmas will also need to be constrained by the numerous SOL measurements to provide as high a fidelity background plasma as possible. Such diagnostics include: core and divertor Thomson scattering, target Langmuir probes, XRCP and MRCP, CER, MDS and filterscopes. With
the constructed backgrounds, DIVIMP will need to be used to understand why little/no methane escaped out of the closed upper divertor, and why MDS was unable to detect it. For discharges where $^{13}\text{C}_{\text{excess}}$ was measured on the collector probes, an analysis similar to that in chapter 4 should be carried out. This future analysis will be of higher fidelity though as the methane experiments have XRCP and MRCP data to constrain the simulated parallel flows (and thus it will no longer be necessary to make assumptions about the magnitude of the parallel flows).

3DLIM should also be used to interpretively model the collector probe deposition patterns similar to that in chapter 3 and 4. The MRCP and XRCP data may be used to constrain the background plasma in 3DLIM. The methane experiment analysis would benefit from a number of 3DLIM upgrades, including but not limited to: importing actual connection lengths, direct-coupling with DIVIMP and a more realistic background plasma prescription (cf. section 4.5). These upgrades are significant, and may in fact justify the development of a new code that makes better use of existing plasma solvers. For instance, a 3D simulation volume may be constructed and instead of applying the simple/complex plasma prescriptions used in chapter 3, SOLPS-ITER could be used to generate a background plasma. This type of approach to the background plasma would be more appropriate than that currently used in 3DLIM since 3DLIM in fact generates plasma solutions starting from target Langmuir probe data (which are generally unavailable in the far-SOL of the collector probes) and interpretively matches upstream MRCP data, whereas SOLPS would effectively start by matching MRCP data without requiring target Langmuir probe data as input. In other words, 3DLIM uses target Langmuir probe data as input, while SOLPS-ITER would use MRCP data as “input”. In the region of the collector probes, MRCP data is all that is available since there are no Langmuir probes on the wall portions that the collector probe field lines limit on, thus a SOLPS-ITER approach may be more appropriate. Such a background plasma could then either be imported into a new 3D Monte-Carlo impurity transport code designed to simulate collector probe deposition patterns, or 3DLIM could be heavily modified to accept a SOLPS-ITER background plasma. The ideas outlined here are a significant undertaking, and should only be undertaken after careful consideration and weighing the risks and rewards of such an approach.
As evident in Fig. 5.9, a significant amount of Mach probe data was taken (over 100 plunges). A database, perhaps associated with the MED, could be compiled and filled with average plasma parameters for each discharge, such as the Greenwald fraction which the data is already plotted against. Relatively simply machine learning concepts, such as principle component analysis, linear regression or a random forest, may be applied to this database to extract relationships between plasma parameters and measured Mach numbers. Key insights in the driving physics behind parallel SOL flows could be elucidated if such a trend were to be discovered.

The analysis of the methane experiment is an ongoing, fluid process. As one spends time delving into the data, unexpected trends may appear in the experimental data that warrants dedicated modelling to answer. For instance, the flow analysis of chapter 4, which is central to this dissertation, was not planned at the outset of MRC, and was only carried out after time spent comparing collector probe deposition profiles. The development of a MED would greatly speed up the data exploration process and lead the way for faster, more efficient insights. Furthermore, continued code development would enable higher fidelity simulations, which in turn would provide increased confidence in the interpretive modelling of methane experiment results.
Chapter 6

Conclusions

This is a dissertation on impurity transport in DIII-D. Impurity transport is a massive field of research, and so the focal point of this dissertation is collector probes. Over the course of this PhD, the research group at University of Tennessee has established itself as a leader in the area of designing and deploying collector probes on DIII-D, enabling the group to carry a critical role in the future of the DIII-D research program. The expertise in utilizing the LAMS system and SOL codes such as DIVIMP and 3DLIM create a cohesive pipeline from experimental measurement to interpretive physics validation.

6.1 Contributions to SOL impurity transport and collector probe interpretation from MRC

MRC was carried out shortly before the start of this PhD, yet it has provided years worth of analysis. Chapter 3 presented a number of general trends observed in collector probe deposition patterns as well as the analysis and modelling performed to interpret them. Section 3.3 contains many of the physics results and interpretations obtained by studying the general characteristics in deposition patterns (as indicated in section 3.3.1). Section 3.3.2 presented an empirical scaling law demonstrating the power entering the SOL and connection length to be the most important factors in how much W deposited on the collector probes (3.3.2). It is understood that $P_{\text{SOL}}$ and $L_{\text{conn}}$ are representative of the
effects of parallel and perpendicular W transport. Larger P_{SOL}, in addition to possibly causing increased target sourcing, could lead to stronger upstream-directed parallel forces on the W ions that encourage leakage from the divertor region. Larger L_{conn} corresponds to a larger plasma volume of which the collector probes collect W ions from. The connection to the radial transport aspect is that a longer connection length means the W ions have more space to transport radially before depositing on a probe face, which on average leads to elevated levels of W density in the SOL region of the collector probes. This is closely connected to the effects of a radially varying L_{conn} studied in section 3.3.4; shorter L_{conn} results in steeper deposition profiles that radially decay faster. Taking the results of these two sections together, it may be conjectured that the most controlling plasma parameter in determining the magnitude and shape of collector probe deposition patterns is the connection length due to its first-order effect on the total deposition and the radial structure of the profiles. In section 3.3.3 the number of λ_{ne}’s was introduced as a metric for distance from the separatrix to explain the variance in the ITF/OTF ratio (3.3.3). When inserted within about 2λ_{ne}’s from the separatrix, ITF/OTF was measured to be > 1, and vice-versa. These results are understood to be evidence for near-SOL W accumulation simply because an accumulation in the modelling is expected to occur in the ITF direction, though further examination of the results showed that it was impossible to distinguish the B_T dependence on the ITF/OTF ratio. Indeed, chapter 4 simulated deposition profiles for two collector probes inserted a similar number of λ_{ne}’s from the separatrix for two similar discharges that had drastically different ITF/OTF ratios, demonstrating that B_T-dependent flows are the most controlling factor in whether or not near-SOL W accumulation is to even occur (summarized in the next section). An additional conclusion from section 3.3.4 is that radial convective transport in 3DLIM best reproduces the sharp decreases in the radial deposition profiles. This is a somewhat novel result, as impurity transport has long been modelled with anomalous diffusion coefficient. These results show that the fundamental nature of diffusion, namely that it acts to flatten out density gradients, makes it unable to reproduce the sharp decrease in the radial structure of the deposition profiles in simulations. The convective radial transport assumption may also have a physical basis, as far-SOL transport has been previously observed to be largely convective in nature (“blobby”), and that the
radial convective velocities required to reproduced deposition profiles in 3DLIM are very close to experimentally measured blob velocities in DIII-D. Diffusive radial transport on the other hand, at least in the far-SOL regions of the collector probes, is not easily justified as collisionality is typically very low in these regions. Finally, section 3.3.4 also showed that a simple SOL prescription in 3DLIM best reproduces the peaking along the edges of the collector probes (3.3.5). This result details the fundamentally 3D nature of interpreting the deposition patterns since it is a result of W ions passing by probe faces and turning around to deposit on the opposite face, all while radially and poloidally transporting across field lines. In summary, the analysis of this chapter adds a few extra puzzle pieces to the still incomplete field of SOL impurity transport, particularly impurity transport in the far-SOL.

6.2 Effect of fast parallel flows on the formation of near-SOL impurity accumulation

The deep-dive comparison between two probes inserted for similar shots during MRC provided indirect evidence of long-hypothesized near-SOL impurity accumulation, predicted nearly four decades ago [42], for the first time. It is shown that the probe inserted for unfavorable $B_T$ collected significantly more W on its ITF side, while vice-versa for the probe inserted for favorable $B_T$. The hypothesis was put forward that the probe inserted for unfavorable $B_T$ collected more W on its ITF side because of the formation of a near-SOL W accumulation. The probe inserted for favorable $B_T$ did not collect more W on its ITF side because near-SOL accumulation may not form in favorable $B_T$ due to expected fast inner-target flows (that are experimentally observed on all tokamaks) “flushing out” accumulation.

DIVIMP simulations of the two respective shots were performed. It was shown that in the simulations with a flow pattern similar to that expected in unfavorable $B_T$, near-SOL accumulation does indeed form. To simulate the favorable $B_T$ flow pattern, additional flows were imposed *ad-hoc* over the plasma background. It was found that a modest addition of $M = 0.3$ additional inner target flows was all that was necessary to prevent near-SOL W accumulation from occurring. The far-SOL W distributions from these DIVIMP simulations
were used to guide the W source specification in 3DLIM. It was found that a W source skewed in the ITF direction was necessary to reproduce the experimentally measured deposition patterns for the probe inserted for unfavorable $B_T$, consistent with the DIVIMP prediction of near-SOL W accumulation. Conversely, for favorable $B_T$, 3DLIM required a W source unskewed towards either direction to reproduce deposition patterns, consistent with the DIVIMP prediction of no near-SOL W accumulation. Taken as a whole, these simulations and collector probe deposition patterns are understood to be the first indirect experimental evidence of near-SOL W accumulation, though only in the unfavorable $B_T$ direction. In the favorable $B_T$ direction, fast inner-target flows largely prevent any accumulation from occurring. In the grand scheme of things, these results demonstrate that SOL modeling of impurity transport must correctly account for background plasma parallel flows, as they can have a first-order effect on the poloidal distributions of impurities.

### 6.3 Further contributions from the methane injection experiments

Chapter 5 described the motivation (5.1) for a dedicated impurity transport/collector probe experiment. It was shown that operating in an USN configuration enables inserting an extra collector probes on the DiMES port. By injecting isotopically enriched methane, $^{13}$C could be treated as a tracer particle for collector probe deposition studies. Using $^{13}$C also enables the use of the various DIII-D spectroscopic systems that are designed to view carbon, such as MDS and CER. A significant amount of preparation was needed for the experiments (5.2). A unique USN shape needed to be developed during DIII-D plasma startup time. An USN plasma with a stable strike point location and a crown that sufficiently extended close enough to DiMES was developed by elongating the plasma downwards. Preliminary analysis was also performed that determined CV was the charge state most likely to accumulate, which in turn dictated what carbon lines to monitor on MDS and CER.

The methane experiments were executed in early 2021 and provided a wealth of data to analyze. Initial analysis of MDS CIV and CV data showed that a statistically significant
The amount of injected methane may not be escaping the divertor region, though this may partially be due to the chosen CV line not being a strong enough line to monitor. CER data suggested that methane was escaping the divertor by observing that the fraction of carbon in the plasma increased some time after the methane puff, though it is still not immediately clear if the increase in carbon is only due to the increase in plasma density during the course of the discharge. The best evidence of methane escaping the divertor region is from NRA and LAMS measurements of the “excess $^{13}$C” deposited on the collector probes. Statistically significant amounts of excess $^{13}$C were measured on the collector probes with NRA and LAMS, though the qualitative shape of the deposition profiles are not completely in agreement. Finally, plunging Mach probe data taken during the experiment reproduced the observation of fast inner target directed flows for the favorable $B_T$ direction, but only in the crown region (i.e. the XRCP). Parallel flows in the crown for unfavorable $B_T$ were mostly stagnant, as expected. MRCP and XRCP also supply valuable $T_e$ and $n_e$ data used to constrain future SOL modelling.

A significant amount of analysis still needs to be performed for the methane experiment data. Some possible research topics are outlined in section 5.4. These include the construction of a local database to organize the methane related data to facilitate analysis (MED), background plasma modelling with SOLPS-ITER instead of OSM-EIRENE, 3DLIM upgrades and continued analysis of the plunging Mach probe data. Construction of a MED would facilitate analysis by storing the results of tedious procedures, such as mapping probe locations to plasma coordinates, as well as provide a centralized area for methane experiment related data. Using SOLPS-ITER to provide a plasma background instead of OSM-EIRENE should be considered since the closed upper divertor includes additional volumetric losses, and possible detachment, that OSM-EIRENE is not fully-equipped to replicate. 3DLIM would benefit from a number of upgrades, such as improved models for the background plasma and more realistic connection lengths. A risk/reward analysis should be carried out to consider if the development of a new, narrower scope collector probe simulation code to replace 3DLIM is warranted. Finally, significant time needs to be spent with the Mach probe data to look for trends in the data. The Mach probe data could provide a starting point for a non-impurity transport study, one that is instead focused on the driving mechanisms behind
B\textsubscript{T}-dependent fast parallel flows. This is still a largely unanswered research question, and the database of L-mode measurements covering various densities and injected power could potentially contribute to this question.

6.4 Final remarks

This dissertation shows the usefulness of collector probes. Collector probes are an extremely simple diagnostic; in their simplest form they are just graphite rods inserted into a plasma. Although, the analysis can be very complex, as reproducing the deposition patterns requires state-of-the-art codes, like DIVIMP and 3DLIM, and the knowledge to run them. When the deposition profiles are the only measurement of an impurity in the SOL they act to ground the SOL impurity transport simulations in experimental reality. This is the nature of interpretive modelling. It is expected collector probes will continue to play a growing role in impurity transport studies in fusion devices due to their relative simplicity and capability to shine light on the still unsolved problem of global impurity transport.
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Appendices
A Procedure for mapping collector probe coordinates to plasma coordinates

Obtaining a measurement at a location along a probe is a first step, but to understand what the measurements mean in regards to the plasma, the measurement location must be mapped to the plasma to essentially figure out how far away from the separatrix it was. To figure this out is a two step (albeit rather lengthy steps) process. Step one is to find the (R, Z) location in the tokamak, dubbed machine coordinates. This has nothing to do with the plasma yet, and only describes a location where the origin is the center of the tokamak, i.e. in the middle of the central solenoid. The next step involves finding the plasma equilibrium using a software called EFIT. This gives the (R, Z) location for the magnetic field lines of the plasma (including the separatrix). The distance that the probe is from the separatrix is then \( R - R_{sep} \). An additional step is to find out the distance from the separatrix at the outboard midplane, or OMP. The OMP is the Z location of the magnetic axis. In Fig. 1, this would be where the plus sign is in the middle of the plasma. This distance, \( R - R_{sep} \) OMP, is useful in comparing against codes, which use the OMP as a common reference point for comparing measurements and diagnostics. How one maps the probe location, or any measurement for that matter, to the OMP will be covered in detail below. A quick note though: As long as one understands the meanings of these measurements locations, the following derivations are not crucial to understanding the rest of this dissertation. This process has not been written down in an easily accessible format to the author’s knowledge, so we wish to document these steps to help anyone else who may find themselves needing to perform this relatively common mapping.

A.1 Steps to get (R, Z) location along a probe

As mentioned, the collector probes were mounted on the midplane reciprocating probe MiMES. MiMES enters the DIII-D vacuum vessel through a port at a 13 degree angle with respect to the R direction. A technical drawing of the MiMES insertion geometry from a bird’s-eye view is shown in Fig. 2. The R values in this drawing are distances from the center
of the tokamak, so the left side is the entrance to the area where the plasma is located. An additional R value that we know ahead of time is the R value of the tip of the MiMES holder, which we denote $R_{probe}$. Fortunately, the Z location of MiMES is constant ($Z=-0.18\text{ m}$), and thus we do not perform any trigonometry to figure out the Z location of a measurement location. A simplified drawing of the MiMES arm is shown in Fig. 3 (not to scale). Here we show $R=0$ to be the center of the tokamak, $R_{probe}$ to be the radial location of the tip of the MiMES holder, and $R_{offset} = R_1$. The angle $c$ is simply

$$c = \sin^{-1}\left(\frac{R_{offset}\sin(13^\circ)}{R_{probe}}\right). \quad (1)$$

A quick disclaimer: All the math in this section is just basic trigonometry, just with quite a few steps.

Now the problem stated again is to determine the $(R, Z)$ coordinate of any location along a probe. The geometry of this problem is shown in Fig. 4 where various angles and distances are defined. This outline schematically represents the geometry of the A probe holder, where the actual A insert, here shown an ”AD” insert, is shown as a grey box (another insert would be a grey rectangle on the top half of this drawing, but it is left out). The orientation of this is still a bird’s eye view, and AD is just a naming convention for this insert to distinguish which side it on; the insert on the other side would be ”AU”. The variable we want to solve here is $R_{meas, AD}$, which is the actual R location of a measurement location along the insert. $l_{AD}$ is the distance from the tip of the insert to the measurement location that we would get from say RBS. $\alpha$, $\beta$ and $\delta$ are just constants from the dimensions of the probe holder that are needed. The angles are color coded. Thus with this information the process of following basic trig to solving for $R_{meas, AD}$ is relatively straightforward, and can be broken up into the following steps:

1. $\delta = \sqrt{\alpha^2 + \beta^2}$
2. $d = \tan^{-1}(\beta/\alpha)$
3. $e = c - d$
4. $R_{AD} = \sqrt{\delta^2 + R_{probe}^2 - 2R_{probe}\delta \cos(e)}$
Figure 1: Typical insertion location of collector probes showing the naming convention used for the three sized probes.

Figure 2: Technical drawing of the MiMES insertion geometry. Note the arm is not parallel to the R axis but rather at a 13 degree offset.
Figure 3: Simplified picture of the MiMES insertion geometry. $R_{\text{probe}}$ and $R_{\text{offset}}$ are known ahead of time.

Figure 4: Insertion geometry of an AD probe insert.
5. \[ f = \sin^{-1}\left(\frac{R_{\text{offset}} \sin(13^\circ)}{R_{AD}}\right) \]

6. \[ R_{\text{meas, AD}} = \sqrt{l_{AD}^2 + R_{AD}^2 - 2l_{AD}R_{AD}\cos(f)} \]

For the other insert, Fig. 5, the process is similar:

1. \[ k = 360^\circ - d - c \]

2. \[ R_{AU} = \sqrt{\delta^2 + R_{\text{probe}}^2 - 2R_{\text{probe}}\delta \cos(k)} \]

3. \[ m = \sin^{-1}\left(\frac{R_{\text{offset}} \sin(13^\circ)}{R_{AU}}\right) \]

4. \[ R_{\text{meas, AU}} = \sqrt{l_{AU}^2 + R_{AU}^2 - 2l_{AU}R_{AU}\cos(m)} \]

For the other B and C probes, we followed a similar procedure. The main difference is that the B probe was at a higher location than the A probe (Z=-0.16 m) and the C probe was lower (Z=-0.21 m).

### A.2 Steps to map an (R, Z) location to distance from separatrix

Once we know the (R, Z) machine coordinates of any location along a probe, we can then proceed to map that location into a distance from the separatrix at either the probe’s Z location, \( R-R_{\text{sep}} \), or at the OMP, \( R-R_{\text{sep}} \) OMP. DIII-D uses the software EFIT to construct the magnetic field line data as shown in Figs. 2.1 and 1. This data can be read using common programming languages, such as Python. This includes the *normalized poloidal flux* of each line, \( \phi_N \). The details of this variables are not relevant here, all that matters here is the \( \phi_N < 1 \) is in the core, \( \phi_N > 1 \) is in the SOL, and \( \phi_N = 1 \) is the location of the separatrix. Thus for each location in the tokamak, EFIT gives us the (R, Z, \( \phi_N \)).

To map a measurement location on the probe, \( (R_1, Z_1) \), to the OMP, \( (R_{\text{OMP}}, Z_{\text{OMP}}) \), we make use of the interpolate module from the scipy package in Python. This uses numerical methods to, for example, create a function of a variable given two input variables. So for this mapping procedure, the steps to map to the OMP were:

1. Create interpolation function \( \phi_N(R, Z) \).
2. Find $\phi_N$ of probe measurement location, $\phi_{N1} = \phi_N(R_1, Z_1)$.

3. Create interpolation function $R(\phi_N, Z)$.

4. Find $R_{OMP}$, which is at $Z_{OMP}$, $R_{OMP} = R(\phi_{N1}, Z_{OMP})$.

5. Find $R_{sep, OMP}$, the R value of the separatrix at the OMP, $R_{sep, OMP} = R(1.0, Z_{OMP})$.

Thus at the end of this procedure we have the probe measurement location mapped to the OMP, which allows us to calculate the key quantity $R - R_{sep}$ OMP for comparing to models. An example to highlight the process: For an AU probe, an W areal density of 0.086 W/cm$^2$ was measured from RBS at 2.1 cm from the tip of the probe. Following the steps for accounting for the 13$^\circ$ insertion angle, this gives machine coordinates of this location, in meters, to be $(R, Z) = (2.310, -0.18)$. From EFIT, this location is $R - R_{sep} = 9.3$ cm from the separatrix. To map to the OMP, we follows our mapping steps and find that at the OMP this measurement location is $R_{OMP} - R_{sep, OMP} = 10.1$ cm from the separatrix. Fortunately, this process was automated using a Python script we wrote.
Figure 5: Insertion geometry of an AU probe insert.
Vita

Shawn Zamperini was born in Virginia Beach, VA in 1993. He graduated from the University of Virginia in 2016 with a B.S. in Physics. In 2020 he received an M.S. in Nuclear Engineering from the University of Tennessee. Shawn is an avid supporter of diversity, equity and inclusion (DEI) efforts in the scientific community, and serves as one of the founding members of the DIII-D DEI panel. Outside of academics he enjoys playing soccer and disc golf, and while at University of Virginia played collegiate Quidditch for 4 years. After his Ph.D. Shawn will start his role as a Staff Scientist at General Atomics, where he will continue working with DIII-D.