MODELING ENHANCED IMPURITY SPUTTERING DUE TO RF SHEATHS IN FRONT OF ICRH ACTUATORS

BY

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THESIS
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Abstract

One of the main concerns over using the Ion Cyclotron Resonance Heating (ICRH) is the enhanced impurity sputtering phenomenon due to the emergence of RF sheaths near the Faraday Screen of the ICRH antenna. Here we present a semi-analytical fluid plasma model able to capture the enhanced sputtering yield from the Faraday Screen and the Plasma-Facing Components of an Ion Cyclotron Resonance Heating antenna in a fusion machine. The model is a one-dimensional phase-resolved model of a rectified radio frequency sheath in a magnetic field at an angle with respect to the material surface, solving for the momentum transport of both the ions and the impurities. The sputtering model of the impurities coming off from the wall is based on lookup tables obtained from the plasma-material interaction code Fractal-Tridyn. This study analyzes a range of magnetic angles and wave frequencies to parametrically investigate their effect on the energy-angle distributions of the impacting ions and sputtered impurities. Finally, an estimate of the impurity fluxes and of the gross-erosion rate is provided for ITER-relevant conditions.
To the man who has never failed me, even when I did not know I needed him.
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Chapter 1

Introduction

1.1 Fusion

1.1.1 Nuclear Reactions

Nuclear energy is the energy released from nuclear reactions that involve the core of the atom. In nuclear reactions a mass difference between the reactants and the products is converted into energy following Einstein's famous equation \( E = mc^2 \). There are two possible types of nuclear reactions that can be harvested as a source of energy: fission and fusion. While fission is the more established and proven commercial power source, radioactive nuclear waste, nuclear proliferation issues and catastrophic nuclear disasters shifted public perception negatively with regard to the usage of nuclear fission power plants. Fusion on the other hand has been hailed as the holy grail of scientific evolution for its promise of a clean and abundant energy source. Fusion releases energy by fusing two nuclei into elements with a smaller total mass. There are several fusion pathways considered for nuclear fusion power plants, note worthy of mentioning are:

\[
2H + ^3He \rightarrow ^4He + ^1H \quad \text{(1.1)} \\
^1H + ^{11}B \rightarrow ^3He \quad \text{(1.2)} \\
2H + ^3H \rightarrow ^4He + n \quad \text{(1.3)}
\]

Nuclear reaction \(1.1\) allows for an aneutronic fusion and can be potentially be a more
efficient way of harvesting energy as most of the energy is carried by charged particles but the lack of $^3\text{He}$ fuel on earth provides a significant hurdle for its commercial use. Nuclear reaction 1.2 provides the same advantages as nuclear reaction 1.1 with an abundance of fuel source but is more technologically challenging as the reactants need to be heated to 123 keV to reach optimum reaction cross sections. Nuclear reaction 1.3 is the easiest nuclear reaction having a cross sectional peak at the lowest energy making it the most suitable fuel for the first generation of nuclear fusion reactors. While Deuterium($^2\text{H}$) can be found naturally in ocean with a weight fraction of $3.12 \times 10^{-5}$, Tritium ($^3\text{H}$) being an unstable nuclei with a half life of 12.3 years faces an abundance problem. A solution to the lack of abundance of Tritium would be the production of Tritium on site by the neutron activation of the blanket breeder material Lithium($^6\text{Li}$).

\[
n + ^6\text{Li} \rightarrow ^3\text{H} + ^4\text{He}
\]  

An added advantage of using nuclear reaction 1.4 to produce Tritium is that it has a positive net energy of 4.8 MeV and can be regarded as an added energy source in fusion reactors. It also provides a technological path for capturing the fusion energy released in nuclear reaction 1.3 and carried by the neutrons (n).

### 1.1.2 Nuclear Cross Section

A nuclear cross section is the probability that a given nuclear reaction will take place. For nuclear reaction 1.3, the cross section is heavily dependent on the energy of the reactants. For a fusion reaction to occur the nuclei must reach a distance in the order of $10^{-15}$ meters so that the strong nuclear force can overcome the repealing coulomb forces between the charged particles. In order for the nuclei to fuse they need to reach very high temperatures to overcome the potential well and reach such short distances. The velocity average nuclear cross section for some of the most notable nuclear reactions is shown in Figure 1.1. To achieve the highest nuclear cross section for nuclear reaction 1.3 the reactants have to be
heated to the temperature $\sim 15K\text{eV}$.

1.2 Controlled Fusion

The atoms for peace conference in Geneva on September 1958 officially declassified the research documents on controlled fusion research, sparking an international collaboration towards the goal of achieving a self sustaining economical commercial fusion power plant. 60 years of strong international collaboration has lead to some noteworthy progress results.
and produced several fusion device designs. The tokamak and stellarator designs are largely backed by the scientific community to be the first generation nuclear fusion power plants. International collaborations for the goal of fusion has manifested itself in the world’s largest fusion experiment ITER. ITER is designed to be the first fusion device to reach the break-even point producing more power than it consumes. To reach break even point ITER will need to heat the plasma to \( \sim 15 \text{ KeV} \). This is achieved using several heating mechanisms including ohmic heating, Radio-Frequency (RF) heating, Neutral Beam Injection (NBI).

### 1.3 Heating

Tokamak design leverages ohmic heating as the initial phase of heating. Changing magnetic fields induce an electric current into the plasma. Plasma resistance is inversely related to the plasma temperature \( \propto T_e^{-3/2} \). This sets an upper limit to the temperatures that can be reached using ohmic heating with high efficiency. After the initial phase of ohmic heating, other methods have to be used to further increase the plasma temperature until it reaches ignition. Ignition is the point when the plasma is self sustaining and no longer requires external heating. RF heating is a strong candidate to help transition from ohmic heating to the point of ignition.

#### 1.3.1 RF Heating

RF waves launched into the plasma are capable of transferring their energy to the plasma through different Wave-Plasma interaction mechanisms. In a tokamak each charged species \( j \) has several characteristic frequencies most important of which are the plasma frequency (\( \omega_{pj} \)) and the cyclotron frequency (\( \omega_{cj} \)). Majority of the energy transfer take place at different resonant frequencies. Choosing a specific resonant interaction by controlling the frequency of the wave gives RF waves the versatility and ability to target specific species. Targeting the Ion cyclotron frequency (\( \omega_{ci} \)) is a method of heating known as Ion Cyclotron Resonance.
Heating (ICRH). ICRH is envisioned as one of the principal strategies of auxiliary heating power for ITER and future commercial fusion reactors from early on [2]. Along with being one of the presently most developed and experimented techniques, it has the advantage of not having a density limit to its applicability. The ICRH technique uses radio-frequency waves in the ion cyclotron range (typically of few tens of mega-hertz) to heat the plasma, by injecting a RF wave into the plasma via an antenna covered by a Faraday Screen (FS) of conductive material. Proper injection of ICRH power requires the ICRH antenna structure to be placed in close proximity to the plasma edge to attain good coupling between the radio waves and plasma. The wave creates an electric field that aligns with motion of the ions throughout the gyro orbit providing constant acceleration for the ions as the wave energy damps out. The process of cyclotron resonance is demonstrated in Figure 1.2. There are two types of waves that can be launched and used to transfer energy into the plasma: the Fast Wave (FW) and the Slow Wave (SW). The latter of which is the one currently being used in ICRH designs. The aim of current ICRH technique is to couple a FW to the plasma where it will propagate to the plasma core and deposit its energy to the ions.

Figure 1.2: Mechanism of cyclotron resonance at the plasma frequency \( \Omega \). Figure from [3]
1.4 Plasma Waves

This section will derive the different type of plasma waves that are relevant for the ICRH technique in order to clarify the distinction between the FW and the SW.

1.4.1 Dispersion Relation

To clarify the difference between the FW and SW we derive the cold plasma dispersion relation starting from Maxwell equations written in phase space with a combined displacement and plasma currents:

\[ i \mathbf{k} \times \mathbf{E} = i\omega \mathbf{B} \]  
(1.5)

\[ i \mathbf{k} \times \mathbf{B} = -i\omega \varepsilon_0 \mu_0 K \cdot \mathbf{E} \]  
(1.6)

Combining equations 1.5 and 1.6 results in the following wave equation:

\[ \mathbf{n} \times (\mathbf{n} \times \mathbf{E}) + K \cdot \mathbf{E} = 0 \]  
(1.7)

where \( \mathbf{n} = \mathbf{k}c/\omega \) is the index of refraction vector with a direction determined by \( \mathbf{k} \) the wave vector. Assuming \( \mathbf{k} \) lies on the x-z plane and the magnetic field \( \mathbf{B} \) only has a constant z component, equation 1.7 can be written in a dispersion relation form \([\mathbf{M}]\mathbf{E} = \mathbf{0}\) as:

\[
\begin{pmatrix}
S - n^2 \cos^2 \theta & -iD & n^2 \cos \theta \sin \theta \\
iD & S - n^2 & 0 \\
n^2 \cos^2 \theta & 0 & P - n^2 \sin^2 \theta
\end{pmatrix}
\begin{pmatrix}
E_x \\
E_y \\
E_z
\end{pmatrix}
= 0
\]  
(1.8)

Where \( S, D \) and \( P \) are stix labels [4]:

\[ S, D, P \]
\[ S = 1 - \sum_{j} \frac{\omega_{pj}^2}{\omega^2 - \omega_{cj}^2} \]  \hspace{1cm} \text{(1.9)}

\[ D = \sum_{j} \frac{\epsilon_j \omega_{cj} \omega_{pj}^2}{\omega (\omega^2 - \omega_{cj}^2)} \]  \hspace{1cm} \text{(1.10)}

\[ P = 1 - \sum_{j} \frac{\omega_{pj}^2}{\omega^2} \]  \hspace{1cm} \text{(1.11)}

Where \(\omega_{pj}\) and \(\omega_{cj}\) are the plasma and cyclotron frequencies defined as:

\[ \omega_{pj} = \sqrt{\frac{n_j q_j^2}{M_j \epsilon_0}} \]  \hspace{1cm} \text{(1.12)}

\[ \omega_{cj} = \frac{q_j B}{M_j} \]  \hspace{1cm} \text{(1.13)}

### 1.4.2 Low Frequency Approximation

ICRH technique operates in a low frequency regime \(\omega \ll \omega_{ci}\), allowing us to approximate the plasma as a perfectly conducting fluid. Approximating the plasma as a conducting fluid is known as the magnetohydrodynamic (MHD) approximation. Assuming a two species plasma of electrons and ions (ie; \(j = e, i\)) equations 1.9, 1.10 and 1.11 can then be simplified as:

\[ S = 1 + \frac{\omega_{pi}^2}{\omega_{ci}^2 - \omega^2} - \frac{\omega_{pe}^2}{\omega_{ce}^2 - \omega^2} \simeq 1 + \frac{\omega_{pi}^2}{\omega_{ci}^2} \simeq 1 + \frac{c^2}{V_A^2} \simeq K_A \]  \hspace{1cm} \text{(1.14)}

\[ D = \frac{\epsilon_i \omega_{ci} \omega_{pe}^2}{\omega (\omega^2 - \omega_{ci}^2)} - \frac{\epsilon_i \omega_{ci} \omega_{pi}^2}{\omega (\omega^2 - \omega_{ci}^2)} \simeq \frac{-\omega c^2}{\omega_{ci} V_A^2} \simeq 0 \]  \hspace{1cm} \text{(1.15)}

\[ P = 1 - \frac{\omega_{pi}^2 + \omega_{pe}^2}{\omega^2} \rightarrow \infty \]  \hspace{1cm} \text{(1.16)}

Where \(V_A^2\) is the alfven wave speed and \(K_A\) is the alfven refraction index. Substituting equations 1.14, 1.15 and 1.16 back into matrix 1.8, we get the Cold Plasma Dispersion
Relation in the MHD approximation:

\[
\begin{pmatrix}
K_A - n^2 \cos^2 \theta & 0 & n^2 \cos \theta \sin \theta \\
0 & K_A - n^2 & 0 \\
n^2 \cos^2 \theta & 0 & \infty
\end{pmatrix}
\begin{pmatrix}
E_x \\
E_y \\
E_z
\end{pmatrix} = 0 \quad (1.17)
\]

Matrix (1.17) can be rewritten in the form of three equations:

\[
(K_A - n^2 \cos^2 \theta) E_x + (n^2 \cos \theta \sin \theta) E_z = 0 \quad (1.18)
\]
\[
(K_A - n^2) E_y = 0 \quad (1.19)
\]
\[
(n^2 \cos^2 \theta) E_x + (\infty) E_z = 0 \quad (1.20)
\]

For the set of equations (1.18), (1.19) and (1.20) there exist only two possible non-trivial classes of solutions:

\[
\begin{cases}
E_z = 0, E_y \neq 0 & \text{if } E_x = 0 \quad (1.21) \\
E_z = 0, E_x \neq 0 & \text{if } E_y = 0 \quad (1.22)
\end{cases}
\]

### 1.4.3 Slow Wave and Fast Wave

Class (1.21) is known as the Slow wave, and class (1.22) is known as the Fast Wave for reasons that will be clarified shortly. Plugging in the two classes of solutions (1.21) (SW) and (1.22) (FW) into equations (1.18), (1.19) and (1.20) gives us the dispersion relation for the two classes of solutions:

\[
\begin{cases}
n^2 \cos^2 \theta = K_A & \text{SW} \quad (1.23) \\
n^2 = K_A & \text{FW} \quad (1.24)
\end{cases}
\]
The dispersion relations $1.23$ and $1.24$ can be used to calculate the phase speed for the SW and FW respectively:

\[
\begin{align*}
\nu_p &= \frac{c^2 \cos^2 \theta}{K_A} = V_A^2 \cos^2 \theta \quad \text{SW} \\
\nu_p^2 &= \frac{c^2}{K_A} = V_A^2 \quad \text{FW}
\end{align*}
\]

As the phase speed of the SW (equation $1.25$) depends on the cosine of the launch angle, there is a range of angles when the phase speed of the SW (equation $1.25$) is slower in comparison with phase speed of the FW (equation $1.26$) hence the naming SW and FW. Figure 1.3 shows the wave normal surface plot of the alfvén waves with the FW having a faster or equal phase speed than the SW at all angles.

### 1.5 Plasma Sheaths

A plasma sheath is a region of space characterized by a net positive charge. The net positive charge in the plasma sheath balances the net negative charge on the surface of the wall in contact with the plasma. The surface material is referred to as the Plasma Facing Component.
Plasma sheaths act as a buffer region between the net negative PFC and a net neutral upstream plasma. Plasma Material Interactions (PMI) happens between the sheath and the PFC. The difference in potential between the net neutral upstream plasma and the net negative PFC creates an electric field that accelerates the ions towards the PFC leading to the heavy ion bombardment of the PFC. Ions impacting the PFC causes the sputtering of neutral impurities that can travel upstream to the core of the plasma unaffected by the electric or magnetic fields. This leads to the heavy element contamination of the plasma, greatly reducing the energy output and stability of the plasma core. Impurity sputtering from the PFC is one of the main issues with fusion technology currently.

1.5.1 RF Sheaths

The close proximity of the biased ICRH antenna combined with the presence of RF waves lead to the emergence of a magnetized radio frequency plasma sheath. The plasma sheaths are mainly driven by radio-frequency voltages and hence known as RF sheaths [6] [7] [8]. The formation of an RF sheath in front of an antenna surface has great implications for the survivability of the Plasma Facing Components of the antenna. A radio frequency sheath exhibits rectified voltages much larger than the local plasma temperature. As a consequence of rectified voltages RF sheath enhanced impurity sputtering and the presence of hot spots [9] have been observed. Self sputtering avalanches due to large sheath potentials have been used to explain large influx of Ni from the FS [10]. The resulting phenomena from large rectified sheath potentials lead to plasma edge power dissipation causing a reduction in heating and RF coupling efficiency well as physical damage to the FS [11]. Understanding and minimizing impurity sputtering from the antenna surfaces is thus of crucial interest to prevent erosion of ICRH surfaces and edge/core contamination.

In theory an ideal use of ICRH should not have interactions with any part of the plasma other than the intended resonance layer for power deposition. In application there are two common physical scenarios that lead to the deviation from ideal: First scenario is when the
FW comes into contact with the PFC structure either because it avoids the scrape-off-layer (SOL) \[12, 13\] or when some of the wave components are not fully absorbed by the resonant layer from a single pass and propagate through to the other inside of the vacuum vessel \[13, 14\]. While the FW by itself does not cause any sheath rectification, Maxwell equations boundary condition dictate that when a FW comes in contact with a boundary surface like the vacuum vessel it couples to a SW upon contact. The second scenario is a more direct launch of a SW into the SOL due to a misalignment between the RF antenna and the magnetic fields. The common physical cause between the two scenarios that leads to the creation of RF sheaths is the emergence of a SW that is in contact with the RF antenna structure. The emergence of RF sheaths is to counter the effect that the SW has on the plasma. The parallel component of the SW RF electric field \(E_{\parallel} = B \cdot E_{RF}/B\) pushes the electrons towards the wall and out of the plasma. The plasma then develops a large rectified sheath potential of the order of several hundred volts pushing the electrons back into the plasma to avoid losing ambipolarity.

Previous experiments on C-MOD \[15, 16\] and on JET \[17, 18\] indicate a correlation between localized enhanced impurity sputtering and the presence of RF-sheath potentials on or around active antennas. Plasma surface interaction experiments on the Faraday screen of JET’s ICRH antenna coated with beryllium, similar to the Faraday screen which will be used for ITER \[19, 20\], observed a significant beryllium influx from optical diagnostics, but never reported an erosion rate. On the other hand, erosion experiments on C-MOD using boron wall conditioning on the antenna surfaces estimated a net erosion rate in the range 15-20 nm/s. Such an estimate would lead to an effective removal of all the boron protective layer in a single 3 MW ICRF discharge operated for only \(\sim 1\) second. Despite the differences in size between C-MOD and ITER, the C-MOD ICRH antennas obtain power fluxes of \(\sim 10\) MW/m\(^2\), in excess of the power fluxes expected on ITER’s ICRH antennas. Assuming a similar erosion rate for Be as the B erosion rate in C-MOD, \(\sim 1000\) discharges (400 discharges/second) would be sufficient to erode through 1 cm of Be coated on ITER’s
Faraday screen [21].

Recent experimental investigations now focusing on the subject of impurity sputtering from such systems [22, 23, 24, 25, 26]. Ample evidence and supporting theories [27] indicate that ICRH antennas enhance the sheath potential on the flux tubes magnetically connected to the antenna surfaces, causing RF sheath potential drops that are significantly greater (of the order of tens to hundreds $T_e$’s) than the classical thermal sheath potential drops ($\sim 3-4 T_e$, depending on the ion mass). This can be traced back to the misalignment between the current straps of the antenna and the perpendicular magnetic field. The misalignment leads to the coupling of the slow wave of the ion cyclotron wave with the plasma, generating a non-zero longitudinal electric field $E_{||} \neq 0$ [28]. In the case of ITER, high power ICRH operation (20 MW) demands that the antenna biased voltage be much larger than the Bohm sheath potential, i.e. $eV_{RF} \gg 3T_e$. This bias behaves similarly to a classical thermal sheath (hence the name rectification), blocking the electrons and accelerating the ions in order to sustain ambipolarity, creating a large rectified direct current (DC) sheath potential in the process. However, differently than classical thermal sheaths, ion accelerations are much larger, and up to hundreds of $T_e$’s, thus potentially causing much more impurity sputtering. Furthermore, the ion dynamics is modulated during each RF cycle. The details of such modulation are extremely relevant for an accurate determination of the ion energy-angle distributions during the RF cycle, and ultimately of the surface response during ion irradiation.

1.6 Plasma Material Interactions

Plasma Material Interactions (PMI) is one of the biggest engineering challenges facing fusion power at the current phase. Interactions between the plasma sheaths and the walls of the vacuum vessel greatly affect the plasma contamination, stability, and energy production. The main concern in the PMI field is the sputtering of wall particles by energetic ions. The sputtered particles are commonly neutral, allowing them to propagate to the center of
the plasma unaffected by the magnetic and electric fields. This gives rise to several plasma instabilities as heavy particles from the wall contaminate the plasma. The sputtered particles are also relatively colder than the plasma causing a quenching effect as they propagate away from the walls. The ability to predict the sputtering yield from the walls due to ion bombardment is crucial for the goal of minimizing the plasma contamination.

1.6.1 Sputtering

The ejection and distortion of particles from the wall material as a consequence of the interactions between the wall material and the energetic ions is known as sputtering. While there are several physical mechanisms for the interaction between the wall material and the bombarding ions, two mechanisms are specifically enhanced during RF operations: Potential sputtering and Kinetic sputtering. As the positively charged ions approach the surface material, they create potential wells near the wall surface that lead to the emission of particles from the wall material. This sputtering mechanism has a strong dependence on the charge of the ions and the target species with insulators exhibiting high potential sputtering. While the charge of ion species is enhanced due to the presence of strong electric fields, the usage of a conducting material as a FS wall severely diminishes the effects of potential sputtering.

Kinetic sputtering, on the other hand, is highly relevant for the scope of this thesis. Momentum exchange takes place due to the collisions between the energetic ions from the plasma and the surface material leading to a collision cascade in the wall material. The cascade of momentum transfer lead to some particles reaching the surface with energies above the surface binding energies allowing them to leave the surface. This is the main physical phenomenon behind kinetic sputtering. Several aspects determine where the energetic ions deposit their energies and the number of atoms that reach the surface with energies larger than the surface binding energy. Most relevant of which are the ion impact energy, the ion impact angle, the roughness of the surface and species involved in the interactions. The focus of this thesis will be on the ion impact angle and the ion impact energies. Kinetic
sputtering starts after a threshold energy below which the ions do not have enough energy to emit any sputtered particles. Above the threshold energy, the number of particles sputtered rapidly increases as the ions have more energy to transfer to the wall material. When the ions start to travel deeper into the material they deposit their energy deep enough that the number of atoms that reach the surface due to the cascade of collisions decreases leading to a decrease in the sputtering yield at very high energies (Visible in Fig 1.4). The ion impact angle also determines the depth at which the ions deposit their energies and hence affects the sputtering yield as well.

### 1.6.2 Sputtering Yield Simulation

The ratio between the incoming particle flux to the flux of sputtered particles from the wall is defined as the sputtering yield. Several methods for sputtering yield calculations have been developed. Most notable of which are the semi-empirical formula for sputtering...
yields developed by Yamamura [29] and computational simulations using Molecular Dynamics (MD) or Binary Collision Approximation (BCA) [30]. While semi-empirical formula are useful in predicting the sputtering yield it lacks the ability to provide detailed information about implementation depth or surface changes. Simulations hence have a clear advantage over semi-empirical formulas. MD simulations on the scale relevant to fusion simulations are more computationally expensive than BCA simulations. The latest of the BCA codes developed to be able to simulate Fractal Surface Roughness effects on sputtering yields is F-Tridyn [31].

Fractal TRIDYN (F-TRIDYN) is a Monte Carlo, Binary Collision Approximation that is based on a previous version of the code TRIDYN used in most sputtering simulations. It includes a model for the fractal surface roughness that play a major role in sputtering yields and energy angle distributions of the sputtered particles. A physical illustration of the model used in F-Tridyn is presented in Figure 1.5. Although fractal surfaces have been implemented in previous codes, implementations used in codes like FTRIM [32] are of the order of $O(N^2)$ operations making them highly expensive to scale. F-Tridyn uses the state of the art implementation that is of the order of $O(N)$ operations where $N$ is the number of points used to make up the fractal surfaces. This makes F-Tridyn highly scalable and suitable for implementation as part of multi-scale simulation efforts. Additionally F-Tridyn ability to output lists such as energy-angle distributions of sputtered particles in Cartesian dimensions gives it an advantage in any coupling activity. The ease of coupling with any plasma simulation or material codes makes it the prime candidate to simulate the effects of high energy ion PMI between the plasma sheath boundary and the FS material.

1.7 Thesis Objective

The main focus of this thesis is further extending the model developed in Myra [8] and provide a semi-analytical model of the RF sheath including impurity generation and transport. The
Figure 1.1: An illustrated depiction of the physical processes modeled in F-TRIDYN. These include reflection, sputtering, surface morphology, damage, mixing, implantation, and layered composition. The two colors, blue and orange, represent two materials whose atoms are mixed by ion-atom and atom-atom collisions.

Figure 1.5: Physical model implemented in F-Tridyn illustrated. Figure from [31]
main plasma species in the RF sheath are treated as in Myra [28], using mass and momentum balances, Boltzmann electrons, and the Poisson equation for the plasma potential. The fluid moments of the ions are then used to sample a population of kinetic ions, treated as computational particles, and obtain ion energy-angle distributions at the wall at the time of impact with the surface. Such distributions are then passed as an input into the sputtering code Fractal-TRIDYN [31], for the calculation of the distributions of sputtered impurities. Among the outputs of the code, Fractal-TRIDYN provides the sputtering yields, the reflection yields, and the energy-angle distributions of the particles emitted by the surface during ion-matter interaction. The kinetic distributions provided by Fractal-TRIDYN have been reduced to their zeroth- and first-order moments (impurity density and impurity fluxes), and used as boundary conditions to a set of fluid equations for the impurity species. Thanks to such a model, we have been able to parametrically study a number of features relevant the ICRH sheaths, namely the effect of the near-wall plasma parameters (wave frequency, magnetic field angle, peak-to-peak RF voltage) on the ion impact energy-angle distributions, sputtering yields, and energy-angle distribution of sputtered impurities. Finally, we have obtained estimates of the average flux of sputtered impurities over one RF cycle and the consequent gross-erosion rate.

1.8 Thesis Overview

Having set the goals of the thesis we proceed in chapter 2 to discuss in detail the theoretical framework and the assumptions made in our model. The derivation of the boundary conditions that capture the rectification effect of the RF sheath and the methods of implementation and coupling to F-Tridyn are also included in Chapter 2. Chapter 3 presents the main results of the paper, including the energy-angle distributions of the impacting ions and of the sputtered impurities along with a proposed explanation behind the physical behaviors for the ions and impurities in the RF sheath. Finally, in chapter 4 we discuss the results
obtained in 3 and calculate relevant erosion rates for comparison with experimental data. Included in chapter 4 is a brief conclusion on the results of the model and possible deployment for future computational projects as well as future improvements that have credible motivation backing their pursuit.
Chapter 2

Methodology

2.1 RF Sheath Impurity Model

In this section we report the equations used to describe the dynamics of the main plasma ions and the impurities released by the wall during an RF cycle. The model is based on a set of one-dimensional phase-resolved fluid equations for the ions and the impurities. Electrons are treated as Boltzmann electrons.

The geometry of the problem is reported in Fig. 2.1. The domain \( x = [0, L] \) starts in proximity to the wall and is pointed along the normal to the material surface. The origin of the reference frame \( x_1 \) is placed at the entrance of the Debye sheath (DS), where the presheath ends and quasi-neutrality is broken. The domain extends up to the point \( x_2 = L \), defined as the entrance of the magnetic presheath (MPS), or the point where the ion flow velocity parallel to the magnetic lines is equal to the Bohm acoustic speed \( C_s \). The simulation domain thus spans from the entrance of the Debye sheath to the entrance of the magnetic presheath, a region where the ion parallel velocity is always supersonic (larger than the Bohm acoustic speed). The Debye sheath is treated as a thin vacuum layer separating the upstream plasma from the wall.

In our model, the 1D equation for local plasma potential with Boltzmann electrons has the form

\[
\frac{\partial^2 \phi}{\partial x^2} = -\frac{e}{\epsilon_0}(Z_j n_j - n_e), \quad (2.1)
\]

\[
\frac{\partial n_e}{\partial x} - \frac{e n_e}{T_e} \frac{\partial \phi}{\partial x} = 0, \quad (2.2)
\]
where $\phi(x,t)$ is the electrostatic potential, $e$ is the fundamental charge, $T_e$ is the electron temperature in energy units (the Boltzmann constant is implicit), and $n_j(x,t)$ is the charge density, where the subscript $j$ stays for ions ($i$), electrons ($e$) and impurities ($I$) respectively, $j = i, e, I$ and $Z_j = Z_i, -1, Z_I$. In the numerical calculations reported in this paper, we have chosen ions to be deuterium ($Z_i = +1$), and impurities to be beryllium ($Z_I = +1, ..., +4$), as per ITER ICRH antenna design specifications [20, 18]. Eqs. 2.1–2.2 are solved with boundary conditions

$$\phi(0,t) = -\frac{V_{pp}}{2} \cos \omega t, \quad (2.3)$$
$$\frac{\partial \phi(L,t)}{\partial x} = 0, \quad (2.4)$$

where $V_{pp}$ is the peak-to-peak amplitude of the oscillating voltage. Sheath rectification is accounted through an additional condition obtained from the current balances across the sheath, discussed in Sec. 2.1.1. The particle densities $n_j(x,t)$ and the electrostatic potential $\phi(x,t)$ are functions of space and time, whereas the electron temperature $T_e$ is assumed to be constant across the simulation domain (isothermal sheath approximation).
The continuity and momentum equations for the plasma ions are

\[ \frac{\partial n_i}{\partial t} + \frac{\partial}{\partial x} n_i u_{xi} = 0 \quad (2.5) \]

\[ \left( \frac{\partial}{\partial t} + u_{xi} \frac{\partial}{\partial x} \right) u_{xi} = -\frac{Z_i e}{m_i} \frac{\partial \phi}{\partial x} - \omega_{ci} u_{zi} \sin \psi \quad (2.6) \]

\[ \left( \frac{\partial}{\partial t} + u_{xi} \frac{\partial}{\partial x} \right) u_{yi} = \omega_{ci} u_{zi} \cos \psi \quad (2.7) \]

\[ \left( \frac{\partial}{\partial t} + u_{xi} \frac{\partial}{\partial x} \right) u_{zi} = \omega_{ci} (u_{xi} \sin \psi - u_{yi} \cos \psi), \quad (2.8) \]

where the velocity vector \( \mathbf{u}_i(x, t) = (u_{xi}, u_{yi}, u_{zi}) \) has components expressed in Cartesian coordinates, and the other symbols are \( \psi \) magnetic angle (defined as in Fig. 2.1 as the angle between the magnetic field and the normal to the surface), \( \omega_{ci} = eZ_i B/m_i \) is the cyclotron frequency, and \( m_i \) is the ion mass. Eqs. 2.1–2.8 form a system of partial differential equations, with boundary conditions given by

\[ n_{i,e}(L, t) = n_L, \quad (2.9) \]

\[ u_{xi}(L, t) = u_o \cos \psi, \quad (2.10) \]

\[ u_{yi}(L, t) = u_o \sin \psi, \quad (2.11) \]

\[ u_{zi}(L, t) = 0 \quad (2.12) \]

where \( n_L \) is the density at the entrance of the magnetic presheath \( (x = L) \), and \( u_o \geq C_s \) is the magnitude of the ion flow velocity at the same location. Most of our analysis have been run selecting \( u_o \) a little larger than the ion acoustic speed, \( u_o = 1.1 C_s \). The tests have revealed that the results are pretty insensitive to the actual values chosen, as long as \( u_o \) is strictly larger than \( C_s \) (Bohm-Chodura criterios), so that numerical instabilities are avoided.

While the integration is performed in physical units, the following non-dimensional units
are convenient, especially for comparisons with results from previous RF sheath models[28],

\[
\hat{x} = \frac{x}{\lambda_D}, \quad \hat{n}_{i,e} = \frac{n_{i,e}}{n_L}, \quad \hat{V}_{pp} = \frac{V_{pp}}{T_e}, \quad \hat{t} = \omega_{pi} t, \\
\hat{u}_j = \frac{u_j}{C_s}, \quad \hat{\phi} = \frac{e\phi}{T_e} \quad \hat{\omega}_{ci} = \frac{\omega_{ci}}{\omega_{pi}}, \quad \hat{\omega} = \frac{\omega}{\omega_{pi}}
\]

where as usual \(C_s = \sqrt{T_e/m_i}\) is the ion sound speed, \(\lambda_D = \sqrt{\epsilon_0 T_e/n_L e^2}\) is the Debye length, and \(\omega_{pi} = \sqrt{n_L e^2/\epsilon_0 m_i}\) is the ion plasma frequency. Most of our results will be expressed using such non-dimensional units. While \(\hat{\phi}\) and \(\hat{V}_{pp}\) only determine the structure of the Debye sheath, the two non-dimensional parameters \(\hat{\omega}\) (degree of ion mobility) and \(\hat{\omega}_{ci}\) (degree of magnetization) considerably affect the physical regimes of the sheath. Their effect will be discussed in 3.2.

Once the plasma ions reach the wall, they interact with the material surface. At the energies of interest in an ICRH sheath, the ions gain enough energy to overcome the surface potential barrier and penetrate into the surface lattice. Once inside the lattice, the ions lose energy mainly via Lindhard-Scharff interaction with the lattice electrons, and in part also via large-angle deflections with the lattice nuclei. Such interactions are responsible for a cascade of effects, all accurately accounted for in the Fractal-TRIDYN code [31].

In the present work we have used Fractal-TRIDYN to produce lookup tables of properties relevant to the RF sheath problem. The lookup tables are publicly available as an open-source dataset at the following permanent url [33]. The properties of interest are the energy-angle distributions of the sputtered particles, the moments of such distributions, and the sputtering yields \(Y_j(E,\theta)\) of the species \(j\). In general, the sputtering yield is a function of the energy \(E\) and the angle \(\theta\) of the incoming ions. The total (effective) sputtering yield \(\tilde{Y}_j(E,\theta)\) is then found from the weighted integral of the sputtering yield \(Y_j(E,\theta)\) over the distribution function \(f_i(E,\theta)\) of the plasma ions,

\[
\tilde{Y}_i = \int \int Y_i(E,\theta) f_i(E,\theta) dE d\theta \quad (2.13)
\]
where the ion distribution \( f_i(E, \theta) \) is assumed to be a drifting Maxwellian of density \( n_i \), temperature \( T_i = T_e \), and drift velocity \( u_i \). The flux of sputtered impurities produced by the wall is then given by

\[
\Gamma_I = Y_i \Gamma_i
\]  

(2.14)

Eq. 2.14 is used as a boundary conditions to the continuity equation of the impurities,

\[
\frac{\partial n_I}{\partial t} + \frac{\partial \Gamma_I}{\partial x} = -\langle \sigma v \rangle_{iz} n_e n_I
\]  

(2.15)

where the right hand side of Eq. 2.15 accounts for sinks of impurities in the plasma due to electron-impact ionization. All sputtered impurities exit the surface as neutral particles, except for some of the alkali metals of the periodic table, like lithium. In the following section, Sec. 2.1.1, we describe in detail the boundary conditions for RF sheath rectification. Additional remarks on the sputtering model will be provided in Sec. 2.3.

### 2.1.1 RF Sheath Rectification

The total current density arriving at the magnetic presheath entrance can be written as the sum of the ion, electron, and displacement currents,

\[
J(L, t) = Z_i e n_i u_{xi} - \mu n_L \cos \psi \exp \left[ \frac{e \phi(0, t) - e \phi(L, t)}{T_e} \right] - \frac{\partial^2 \phi_L}{\partial t \partial x}
\]  

(2.16)

where \( J(L, t) \) is the total current density at \( x = L \) and time \( t \), \( T_e \) is the electron temperature, and \( \mu = -e v_e / \sqrt{2\pi} \) is a modified electron collision frequency. In order to avoid violating conservation of charge during one RF cycle, the total current entering the magnetic presheath at phase \( \omega t \) must be equal and opposite to the total current at phase \( \omega t + \pi \),

\[
J(L, \omega t) + J(L, \omega t + \pi) = 0.
\]  

(2.17)
As a consequence of Eq. 2.17, the total current integrated over one RF cycle must be equal to zero, expressing the fact that there is no build-up of charge during one cycle. Indicating the time-average over one RF period with angle brackets, we get that the ion flux results equal to

\[ \langle n_i u_{xi} \rangle = n_L u_o \cos \psi, \]  

(2.18)

and that the time-averaged displacement current vanishes to zero, \( \langle \partial^2 \phi_L / \partial t \partial x \rangle = 0 \). The time-average \( \langle J(L, t) \rangle \) of the total current density (Eq. 2.16),

\[ \langle Z_i e n_i u_{xi} \rangle - \langle \mu \cos \psi n_L \exp \left[ e(\phi(0, t) - \phi(L, t)) \right] \rangle - \langle \partial^2 \phi_L / \partial t \partial x \rangle = 0 \]  

(2.19)

immediately returns an expression independent than the ion density and the magnetic angle,

\[ \exp \left[ e(V_{pp} \cos \omega t - \phi(L, t)) \right] = \frac{u_o}{\mu}, \]  

(2.20)

which can be further simplified into a boundary condition of the rectified potential at the magnetic presheath entrance,

\[ \phi(L, t) = \frac{T_e}{e} \ln \left[ \frac{\mu}{u_o} \cosh \frac{eV_{pp} \cos \omega t}{T_e} \right] \]  

(2.21)

Eq. (2.21) is used as a boundary condition on the potential at the magnetic presheath entrance \( x = L \) together with the two other conditions Eqs. (2.3) and (2.4).

### 2.2 RF Dispersion Relation

The dependence on periodic boundary conditions discussed in 2.1.1 gives rise to sheath-driven wave behavior in the solutions for Eqs. 2.1–2.2 and 2.5–2.8. To grasp a better understanding on the wave-type behavior we performed a linear dispersion analysis on Eqs. 2.1–2.2 and 2.5–2.8 described in detail in this section. We start our analysis by listing the
assumptions used:

- The parameters $\phi, n_{i,e}, u_{xi,yi,zi}$ were split into two components: A time dependent component denoted by overhead tilde ($\tilde{\phi}, \tilde{n}_{i,e}, \tilde{u}_{xi,yi,zi}$), and an equilibrium component denoted by ($\phi_0, n_{i0,e0}, u_{x0,y0,z0}$). i.e;

$$\phi(x,t) = \tilde{\phi}(x,t) + \phi_0(t) \tag{2.22}$$
$$n_{i,e} = \tilde{n}_{i,e}(x,t) + n_{i0,e0}(t) \tag{2.23}$$
$$u_{xi,yi,zi} = \tilde{u}_{xi,yi,zi}(x,t) + u_{x0,y0,z0}(t) \tag{2.24}$$

- The equilibrium densities are assumed to be independent of time or space taken at the upstream plasma value $n_L$ i.e;

$$\hat{n}_{i0} = \hat{n}_{e0} = n_L \tag{2.25}$$

- The equilibrium velocity components are taken be negligible. We are neglecting any background flow by using this approximation, i.e;

$$u_{x0} = u_{y0} = u_{z0} = 0 \tag{2.26}$$

The result of the plugging in assumptions 2.22–2.26 into Eqs. 2.1–2.2 and 2.5–2.8 followed
by the linearization of the equations is the following set of linearized algebraic equations:

\[-k^2 \tilde{\phi} = -\frac{e}{\epsilon_0} (\tilde{n}_i - \tilde{n}_e) \quad (2.27)\]

\[\tilde{n}_e - \frac{en_L}{T_e} \tilde{\phi} = 0 \quad (2.28)\]

\[\omega \tilde{n}_i - kn_L \tilde{u}_{xi} = 0 \quad (2.29)\]

\[i \omega \tilde{u}_{xi} = -\frac{e}{m_i} ik \tilde{\phi} - \omega_{ci} \tilde{u}_{zi} \sin \psi \quad (2.30)\]

\[i \omega \tilde{u}_{yi} = \omega_{ci} \tilde{u}_{zi} \cos \psi \quad (2.31)\]

\[i \omega \tilde{u}_{zi} = \omega_{ci} \tilde{u}_{xi} \sin \psi - \omega_{ci} \tilde{u}_{yi} \cos \psi \quad (2.32)\]

The resulting dispersion relation from Eqs. 2.27–2.32 can be written as:

\[n_L T_e e^2 \cos^2 \psi k^2 \omega_{ci}^2 + m_i n_L e^2 \omega^4 + m_i \epsilon_0 T_e k^2 \omega^4 =\]

\[n_i T_e e^2 k^2 \omega^2 + m_i n_L e^2 \omega^2 \omega_{ci}^2 + m_i \epsilon_0 T_e k^2 \omega^2 \omega_{ci}^2 \quad (2.33)\]

In most ICRH applications the wave frequency is adjusted to match the ion cyclotron frequency. Assuming \(\omega = \omega_{ci}\) Eq. 2.33 then becomes:

\[k^2 \omega_{ci}^2 (1 - \cos^2 \psi) = 0 \quad (2.34)\]

In such situation the type and existence of a solution highly depends on the magnetic field angle \(\psi\). In the case of a parallel magnetic field (\(\psi = 90^\circ\)), no solution exists for the given model under any set of parameters. This was noticed as the simulations tended to fail when \(\psi \approx 90^\circ\) regardless of the implementation or discretization parameters. The case of the model failure can be attributed to the Maxwell-Boltzmann approximation used for the electrons valid when \(\omega L_x < v_{t} \cos \psi\). At large \(\psi\), the Maxwell-Boltzmann approximation constraint \(\omega L_x < v_{t} \cos \psi\) no longer holds. A second case of interest is in perpendicular
magnetic field angle $\psi = 0$ where Eq. 2.34 yields the result $k = 0$. Physically this represents the case when the wavelength of the wave behavior in the solutions approaches inf and no wave behavior emerges in perpendicular magnetic fields. For $0^\circ < \psi < 90^\circ$ solutions exist with varying wave behavior contributions increasing as the magnetic field approaches parallel angle ($\psi \to 90^\circ$).

### 2.3 Remarks on the Sputtering Model

An important component of the current model is the inclusion of sputtering yields $Y_i(E, \theta)$ calculated using the Fractal-Tridyn code\[31\] (abbreviated as F-Tridyn). In this section we report few remarks on the procedure used to couple F-Tridyn data in the current RF sheath model.

Each Monte-Carlo run of F-Tridyn requires two main type of inputs: (1) atomic and material properties of both the impacting particles and the material surface, (2) the energy-angle distributions $f_i(E_i, \theta_i)$ of the plasma ions impacting on the material surface. In order to pass information from the fluid model of the RF sheath to the kinetic model of F-Tridyn, a fluid-to-kinetic conversion is required. We convert the fluid moments (energies and fluxes) produced by the RF sheath model into kinetic distributions by means of the following simplified approach. The ion impact energy $E_i(t)$ at a time $t$ is given by the sum of two components, fluid energy $E_{fi}$ and thermal energy $E_{th}$,

$$E_i(t) = E_{fi}(t) + E_{th} = \frac{1}{2} M_i \mathbf{u} \cdot \mathbf{u} + \frac{3}{2} T$$

(2.35)

where the ion drift velocity $\mathbf{u} = \mathbf{u}(0, t) = (u_{ix}, u_{iy}, u_{iz})$ is the fluid velocity at a generic time $t$ and spatial location $x = 0$ (wall) obtained from the solution of problem Eqs. (2.6)–(2.8).

The ion impact angle $\theta_i$ is obtained from

$$\cos \theta_i = \frac{v_{ix}}{\sqrt{v_{ix}^2 + v_{iy}^2 + v_{iz}^2}}$$

(2.36)
where the particle kinetic velocity \( \mathbf{v} = (v_{ix}, v_{iy}, v_{iz}) \) has each component given by the sum of drift velocity \( \mathbf{u} \) plus a random thermal component, \( v_{ij} = u_{ij} + v_{th} \cdot r_j \), with \( v_{th} = \sqrt{2T/M_i} \) the most probable speed, and \( r_j \) three normally-distributed random numbers along the three Cartesian directions \((j = x, y, z)\). The distribution \( f_i(E_i, \theta_i) \) of the ions impacting on the surface is then reconstructed from a drifting Maxwellian of temperature \( T \) and drift velocity \( \mathbf{u}(0, t) \) by sampling a large number \((\sim 10^5 - 10^6)\) of computational particles, binning them into bins of \(3^\circ\) along the angular coordinate spanning over the interval \([0^\circ, 90^\circ]\), and finally passed as an input to F-Tridyn.

F-Tridyn then produces a list of sputtered particles (impurities) each with their respective sputtered energy and angle. The distributions of sputtered impurities are reconstructed via a two-dimensional histogram in the energy-angle space. From the moments of the distributions, the boundary conditions to the fluid problem of Eqs. (2.14)–(2.15) are found.

While direct code coupling with F-Tridyn is possible, and explored in a previous work \[34\], F-Tridyn simulations are computationally expensive at energies larger than \(>300\) eV. The computational cost and the process of recalculating the sputtering yield for the same set of input parameters makes it more efficient to produce a dataset in the form of a lookup table. We produced a dataset covering ion energies from \(0 - 1000\) eV with \(10\) eV intervals. We used linear interpolation for data points between intervals to refine the dataset. The code then post-processes the dataset produced to extract the relevant distributions. Post-processing is done as follows. First, the energy and angle of sputtered particles produced by F-Tridyn for a given incoming ion impact energy \(E_i\) and angle \(\theta_i\) are binned creating three normalized velocity distributions, \(\hat{f}_{v_x}(E_i, E_s, \theta_i, \theta_s)\), \(\hat{f}_{v_y}(E_i, E_s, \theta_i, \theta_s)\), \(\hat{f}_{v_z}(E_i, E_s, \theta_i, \theta_s)\), and one angular distribution, \(\hat{f}_{\theta_s}(E_i, E_s, \theta_i, \theta_s)\). The normalized distributions are function of four arguments: \(E_i\) and \(\theta_i\), energy and angle of the incoming ion, and \(E_s\) and \(\theta_s\), energy and angle of the sputtered particle. Then, the sputtering yield produced by F-Tridyn is similarly binned in the two-dimensional plane \((E_i, \theta_i)\) to produce a sputtering yield distribution, \(Y(E_i, \theta_i)\). The dataset produced with F-Tridyn has been made available on Figshare \[33\].
The distributions of the sputtered particles at a generic time \( t \) during the RF cycle is found from a weighted integral of \( \hat{f}_{\theta_s} \) with \( \hat{f}_i(\theta_i) \) at a fixed energy \( E_i \) of the incident ion,

\[
\hat{f}(E_s, \theta_s) = \int \hat{f}_{\theta_s}(E_i, E_s, \theta_i, \theta_s) \hat{f}_i(\theta_i) d\theta_i
\]  

(2.37)

The time-dependent value of the sputtering yield is found in a similar way, from a weighted integral of \( f_Y(E_i, \theta_i) \) with \( \hat{f}_i(\theta_i) \) at fixed \( E_i \),

\[
\bar{Y}(t) = \int Y(E_i, \theta_i) \hat{f}_i(\theta_i) d\theta_i
\]  

(2.38)

From Eq.(2.38) a time-dependent sputtering yield can be obtained during the RF cycle, as will be presented and discussed in Chapter 3.

2.4 Numerical implementation

The model presented in the previous sections (2.1, 2.1.1, 2.2 and 2.3) has been numerically discretized and implemented in a Matlab code. The routines are maintained on a private Git repository at the University of Illinois and are freely available upon request. In this section we briefly describe the numerical methods adopted for the discretization.

The equations of the electric potential, Eqs. (2.1)–(2.2), together with the boundary conditions of Eqs. (2.3), (2.4) and (2.21), are solved by finite-differentiation of the Laplace operator and by means of a Newton-Raphson scheme for the nonlinear term deriving from the Boltzmann electrons. The system of equations Eqs. (2.9)-(2.12) expressing the ion continuity and momentum is discretized using an explicit upwind scheme, and integrated in time until the solution relaxes to a periodic state over several RF cycles. Simulating a small number of RF Cycles does not achieve adequate relaxation and significantly overestimates the ion densities at the FS Wall. On the other hand, a large number of RF cycles amplifies the numerical errors leading to the failure of the simulation, while being computationally expensive. The
number of grid points necessary to a successful simulation varies depending on the problem parameters $\omega, \psi, \omega_{ci}$. In order to achieve convergence and relaxation to a periodic solution, tuning of the discretization parameters is required, namely: number $N$ of spatial grid points, number $M$ of points per RF cycle, total number of RF Cycles, simulation domain size $L$.

The procedure used for the implementation of the numerical method was the following. First, we solved the RF sheath model of Sec. 2.1 model using the initial conditions:

$$\phi(x, 0) = \frac{T_e}{e} \ln \left[ \mu \cosh \frac{eV_{pp}}{2T_e} \right]$$

(2.39)

and initial moments

$$n_{i,e}(x, 0) = n_L,$$

(2.40)

$$u_{xi}(x, 0) = u_o \cos \psi,$$

(2.41)

$$u_{yi}(x, 0) = u_o \sin \psi,$$

(2.42)

$$u_{zi}(x, 0) = 0$$

(2.43)

A typical simulation had to run for at least 10 RF cycles in order to converge to a periodic solution in time.

Good agreement of our implementation with previous literature results has been obtained. Fig. 2.2 shows an example of comparison of our model with previous literature results reported in Myra and D’Ippolito [28]. Furthermore, the size of the Debye sheath of $\sim 10\lambda_D$, defined by the violation of quasi-neutrality ($n_i \neq n_e$), was found to be equal to the values reported in Myra and D’Ippolito [28]. Finally, the magnetic presheath was observed to disappear in regimes of weak ion mobility ($\hat{\omega} = 9$) and magnetic field perpendicular to the wall ($\psi = 0^\circ$), in agreement with previous literature Myra and D’Ippolito [28]. In such conditions, the Bohm-Chodura [35] criterion and the classical Bohm sheath criterion are equivalent, and hence a MPS does not emerge. All the simulations presented in the
next section Results Sec.3 are performed in conditions of low ion magnetization parameter, \( \hat{\omega}_{ci} = 0.1 \). The effects of ion magnetization \( \hat{\omega}_{ci} \) have been previously discussed\cite{28}; here we will focus on characterizing the effect of the RF sheath on impurity production.
Figure 2.2: Comparison of the current model with the model presented in Myra and D’Ippolito [28], for the case of a single-species plasma having normalized parameters $\hat{\omega} = 9$, $\hat{\omega}_{ci} = 1$, $V_{pp} = 20$ and $\psi = 0^\circ$. 
Chapter 3

Results

3.1 Overview

The major goal of the analysis presented in this work is characterizing the sputtering behavior of a material wall interfaced with a radio-frequency sheath. The computational results presented in this chapter summarize few quantitative simulations aimed at providing a general picture of the surface response under a range of conditions relevant for ICRH and LH radio-frequency actuators. Since the sputtering behavior is tightly connected to the macroscopic structure of the plasma sheath, first we outline the behavior of plasma density (both $n_e$ and $n_i$), ion drift velocity, and electric potential as a function of the RF cycle, as obtained from the numerical solution of the model in Chapter 2. Then, the calculated energy-angle distributions of the ions impacting on the wall are analyzed in detail, showing the dependence of the ion energy and the ion impact angle as a function of the RF phase. Finally, the energy-angle distributions of the sputtered particles are presented. From their moments, the flux of impurities released by the wall during a RF cycle are obtained, and used to estimate the amount of impurities released by the surface per each RF cycle.

The simulations reported here cover a range of magnetic field angles from normal incidence to grazing incidence, and equal to $b_x = 1.0, 0.6, 0.2$ (they are equivalent to magnetic angles $\psi = 0^\circ, 53.13^\circ, 78.45^\circ$, with $\psi$ as defined in Fig. 2.1) covering different MPS conditions, going from an absent MPS to MPS larger than the DS. A peak-to-peak normalized voltage $\hat{V}_{pp} = 200$ was used in all simulation cases as it is expected to be relevant for actual fusion operation in ITER (electron temperature $T_e$ of the order of 3 eV and wall bias voltages
of $V_{pp} = 600$ V). While we simulated a wide range of ion mobility $\omega = 0.07, \ldots, 400$, most of our analyses was focused on $\omega = 0.3, 1.0, 9.0$. These three cases cover the different physical regimes and sheath structures, going from highly mobile ions to highly immobile ions.

The organization of the sections is the following. In Sec. 3.2 we report a brief description of the main features of the RF sheath observable from our model. The impact angle distribution and the impact energy of the ions on the FS wall at different times during a RF cycle are presented in Sec. 3.4 and Sec. 3.3 respectively. Sec. 3.5 discusses the resulting Energy-Angle distributions of the sputtered particles under different physical conditions. Sec. 3.6 and Sec. 3.7 deal with the first order moment (particle fluxes) of the distribution of sputtered particles.

### 3.2 Sheath Structure

While the structure of a RF sheath is similar to a classical sheath in its constituents, several differences distinguish a RF from a classical sheath. Fig. 3.1 emphasizes the major features of the sheath structure that are evident with large $V_{pp}$. The figure shows a typical solution from the model described in Chapter 2. The presence of a rectified potential is the main physical phenomenon that leads to changes in sheath structures. Comparing the average potential upstream $\langle \phi(L) \rangle \sim V_{pp}/2$ with the potential in classical sheath cases $\langle \phi(L) \rangle \approx 3$ V gives a clear indication for the presence of DC voltage rectification. During large parts of the RF cycle, the instantaneous upstream potential $\phi(L,t)$ (derived in Eq. 2.21) is significantly higher than the wall potential $\phi(0,t) = -V_{pp} \cos(\omega t)/2$. As a consequence of sheath rectification, large potential drops appear during periods of high negative wall voltage, as seen in Fig. 3.1 (d). As a result of larger potential drops, the electron density $n_e$ is stripped away during most of the RF cycle creating a sheath that is almost devoided of electrons. There exist however periods during the RF cycle (centered around $\omega t \sim \pi$) where the potential drop is significantly smaller, reaching potential drops sufficient to create a more standard thermal
sheath.

The presence and size of a MPS is highly affected by the magnetic field angle $\psi$ as the MPS has to support a potential gradient that is able to accelerate the ions from $u_x = c_s \cos \psi$ at the entrance of the MPS to the entrance of the DS given by the Bohm condition $u_x \geq c_s$. In cases of a perpendicular magnetic field ($\psi = 0$) the entrance of the MPS and the entrance of the DS coincide ($u_x = c_s \cos \psi = c_s$) leading to the absence of a MPS. The presence of a MPS is detected when a large drop in ion density is visible in the MPS region.

The ions are accelerated throughout the DS reaching the FS wall with hypersonic ion normal speeds and higher impact energies. During the periods of large potential drop, the ion dynamics in the sheath is dominated by rectification physics as the effect of electric field force on the ion trajectory becomes much larger than the Hall force acting on the particle.

### 3.3 Ion Impact Energy as a Function of RF Cycle

The ion energy at the time of impact with the wall is a quantity of utmost importance in determining the sputtering response of the surface. Differently than a classical thermal sheath, in a RF sheath the ion energy changes as a function of the RF cycle. Such change in energy has dramatic consequences to the sputtering behavior, since in most of the cases of relevance, the values of the energy fall within a range where the sputtering yield has exponential variations. This leads to a strongly nonlinear response of the impurity release as a function of the RF Cycle.

Fig. 3.2 (top) shows the change in the ion impact energy vs. time during one RF cycle. For reference, we added the RF voltage to the plot (dark red curve), with the lowest voltage occurring at $\omega t = 0$. The figure shows that ion impact energy exhibits strong nonlinear oscillations as a function of the RF phase. When the wall is negatively biased, the ion peak energy is of the order of the total peak-to-peak voltage plus the thermal kinetic component $V_{pp} + E_k$ ($\sim 610$ V in this example). The ion energy then rapidly decreases during the positive
Figure 3.1: Profiles of the simulated normalized physical parameters in an RF sheath for the case $\psi = 78.46^\circ, \hat{\omega} = 0.5, \hat{\omega}_{ci} = 0.1, \hat{V}_{pp} = 200$. Top left (a) ion density $\hat{n}_i$, Top right (b) electron density $\hat{n}_e$, Bottom left (c) ion velocity normal to the wall $\hat{u}_{xi}$, Bottom right (d) electrostatic potential $\hat{\phi}$. The FS is at $\hat{x} = 0$ and time $\omega t$ is advanced in the direction receding to the left of the page.
wall bias phase of the RF cycle. Such strong nonlinear oscillation is quite sensitive to the ratio \( \dot{\omega} = \omega / \omega_{pi} \) (RF frequency over ion plasma frequency). In fact, as the wave frequency \( \omega \) increases with respect to the ion plasma frequency \( \omega_{pi} \), the effect of the ion inertia becomes evident, effectively reducing the ion mobility across the sheath. At low frequency the ions have more time to respond to the changing voltage. Higher frequencies lead to a delayed and more flat response of the energy gain. Two main features are evident from Fig 3.2 (top). The first is a smoothing of the ion impact energy as a function of time, leading to a decrease in magnitude of the peak of impact energy. The second is a shift in the ion peak energy towards the center of the RF cycle, towards \( \omega t \sim \pi \). Indeed, ions in higher mobility regimes tend to respond faster to a variation in RF voltage. An increase in \( \dot{\omega} \) leads to a significant decrease in impact energy during the first half of the RF cycle, with the overall effect of spreading the energy uniformly throughout the RF cycle. In conditions of very low ion mobility (\( \dot{\omega} > 10 \)) the ion impact energy remains almost constant across the whole RF cycle.

The nonlinear oscillation of the ion energy during the RF cycle has deep consequences on the sputtering behavior. Fig. 3.2 (bottom) shows the sputtering yield as a function of time along the same time coordinate, calculated for beryllium (sputtering threshold of \( E_{th} = 12.6 \) eV). Strong nonlinear oscillations on the yield are clearly evident from the plot. At low frequency, \( \dot{\omega} = \omega / \omega_{pi} < 1 \), the ions spend a considerable percentage of the RF cycle below the sputtering threshold. The increase in the impact energy at the start of the RF cycle does not compensate the significant decrease in impact energy for the rest of the cycle. The decrease in impact energy leads to a sharp fall in sputtering yield after the first quarter of the cycle. On average during one RF cycle, at low frequency fewer impurities are sputtered from the surface, with consequences that will be further analyzed in Sec. 3.6. Surprisingly, the sputtering yield at high frequency, \( \dot{\omega} > 1 \), is not much smaller than the low frequency case. In fact, while ions at high frequency do not achieve the same high impact energy of the low frequency case, they spend larger fractions of the RF cycle above the sputtering threshold,
with an overall higher contribution to the yield. The condition $\tilde{\omega} = \omega/\omega_{pi} \approx 1$ (purple curve) represents a regime where the RF frequency approaches the ion plasma frequency. This regime is of most practical interest, as that is the range of frequency that ITER RF launchers will be operating. In such conditions, the behavior is intermediate with respect to the two extreme conditions of high and low frequency. A significant delayed decrease of the sputtering yield of more than one order of magnitude occurs during the positive portion of the RF cycle. Such decrease is not as shallow as in the low frequency case, but enough to quantitatively decrease the average sputtering yield over one RF cycle.

### 3.4 Distribution of Impact Angles

The angular distributions of the impacting ions on the FS wall greatly affects the sputtering yield. Competing forces (electric field force, Hall force, and $E \times B$ drift) that are a nonlinear function of the RF cycle phase and the operational parameters (magnetic angle $\psi$, normalized wave frequency $\tilde{\omega}$) dictate the impact ion angular distribution. This creates a strong dependence for the ion impact angle distribution on the RF cycle phase and the operational parameters that could lead to extreme changes in the ion impact angle distribution, from a perpendicular incidence to a back flow of ions in some cases. Such extreme changes in ion impact angle distributions lead to drastic changes in sputtering yield and the energy-angle distribution of sputtered particles. As a consequence, moments of the sputtered particles flux heavily depend on the RF cycle phase and the operational parameters.

Fig. 3.3 shows the normalized impact angle distributions resulting from the relevant physical regimes at different times during a RF cycle. Four cases are shown: (a) magnetic field perpendicular to the surface at low RF frequency ($\psi = 0^\circ, \tilde{\omega} = 3$), (b) magnetic field perpendicular to the surface at high frequency ($\psi = 0^\circ, \tilde{\omega} = 3$), (c) magnetic field inclined at an angle with respect to the surface at low frequency ($\psi = 78.46^\circ, \tilde{\omega} = 0.3$), and (d) magnetic field inclined at high frequency ($\psi = 78.46^\circ, \tilde{\omega} = 3$). Each plot shows four snapshots of the
Figure 3.2: Ion Impact energy (top) and Sputtering Yield (bottom) for varying $\omega$ for the case $\psi = 0^\circ$, $\tilde{\omega}_{ci} = 0.1 (\omega_{pi})$, $V_{pp} = 200 (T_e)$ for Be. Top Ion Impact Energy, Bottom Sputtering Yield.
angular distribution at four phases of the radio-frequency cycle \((\omega t = 0, \pi/2, \pi, 3\pi/2)\). The figures show the strong dependence that the ion impact angle distribution exhibit on the the RF cycle phase and the operational parameters.

Fig 3.3 (a) (top left) shows the case when the magnetic field is perpendicular to the surface with a low normalized wave frequency \((\psi = 0^o, \hat{\omega} = 0.3)\). At the start of the RF cycle \(\omega t = 0\) the ion impact angle distribution has a sharp bell curve shape around a perpendicular impact angle. The presence of large potential drops creates strong electric fields normal to the wall that dictate the ion trajectory. The electric field tends to form at normal angles with the wall, hence the inclination of the magnetic field determines the role that the \(E \times B\) drift plays. In perpendicular magnetic fields the \(E \times B\) is identically equal to zero as the magnetic and electric fields are parallel. In the absence of an \(E \times B\) drift, the only effect the magnetic field has on the impact angle is due to the induced ion gyro-motion from Hall force effects. As the potential drops decreases when the RF cycle advances, the ion velocity normal to the wall also decreases. With a decreased ion normal velocities the Hall force on the ions starts to have a clear effect on the impact angle causing a small spread in the distribution at times \(\omega t = \pi, 3\pi/2\). In high wave frequency case \((\psi = 0^o, \hat{\omega} = 3)\) (Fig 3.3 (b) (top right)), the ion velocity normal to the wall experience a smaller decrease in value remaining well above supersonic speeds. Such a behavior is expected as the ion impact energy oscillations during a RF cycle greatly decrease with increasing \(\hat{\omega}\), a feature that was discussed in Sec. 3.3. When the ion normal velocities remain well above supersonic speeds the impact angle distribution is largely unaffected by the time of the RF cycle as the ion trajectories in the DS are unaffected by Hall force throughout the RF cycle.

The steep inclination of the magnetic field gives rise to an \(E \times B\) drift that plays a dramatic role in the trajectory of impacting ions. Fig 3.3 (c) (bottom left) show the case of an inclined magnetic field with respect to the surface and a low wave frequency \((\psi = 78.46^o, \hat{\omega} = 0.3)\). The presence of an \(E \times B\) drift affects the impact angle distribution in two noticeable ways: shifting the ions away from a perpendicular impact angle and increasing
the effect of the Hall force on the ion trajectories. The former change can be explained by the change in ion path before impact that the $E \times B$ drift makes. When the magnetic field becomes more oblique deviation from normal ion impact angles created by $E \times B$ drift increases. The latter change can be explained by the increased role that the Hall force plays in more oblique magnetic field cases. The ion guiding center tends to follow a path closer to the magnetic field lines. The change in path creates a deviation in the impact angle distribution center that is directly related to the magnetic field angle. The increased role the ion gyro motion plays with increased magnetization causes the impact angle distribution to disperse without a major shift in the distribution center. The combination of the physical phenomena listed above creates a heavily amplified effect on the impact angle distribution.

At time $\omega t = \frac{3\pi}{2}$ when the Hall force is at its peak, a fraction of the ion particles glaze of the surface without physically impacting the wall, but creating a backward flux of ions that propagate towards the plasma, as can be seen in Fig. 3.3 from the shift in the distribution beyond $\theta_i = 90^\circ$. Although such back flow of ions does not create a major change to the overall sputtering yield, this physical phenomenon raises major interest in possible uses of this method and has considerable potential in future research operations.

### 3.5 Energy-Angle Distribution of the Sputtered Particles

The energy-angle distribution of the sputtered particles dictates the kinetics of how the impurities leave the surface and flow back into the SOL. Changes in the energy-angle distribution could make a difference between prompt local redeposition, or contamination of the upstream plasma and potentially of the core. As a consequence of the dependence of energy-angle distribution of the sputtered particles on the ion impact angle distribution and ion impact energy, operational parameters (magnetic field angle $\psi$, normalized wave frequency $\tilde{\omega}$) drastically affect the sputtering response of the surface.
Figure 3.3: Ion impact angle distribution for the case $\dot{\omega}_{ci} = 0.1$ ($\omega_{pi}$), $\dot{V}_{pp} = 200$ ($T_e$) at times $\omega t = 0, \pi/2, \pi, 3\pi/2$. Top left case a ($\psi = 0^\circ, \dot{\omega} = 0.3$), Top right case b ($\psi = 0^\circ, \dot{\omega} = 3$), Bottom left case c ($\psi = 78.46^\circ, \dot{\omega} = 0.3$), Bottom right case d ($\psi = 78.46^\circ, \dot{\omega} = 3$)
Fig. 3.4 shows the Energy-Angle distribution for different operational parameters at time \( \omega t = \pi \) when the Hall forces on the ions are relevant. Figure 3.4 shows the sputtered impurity energy-angle distribution for four different cases: (a) an inclined magnetic field at low frequency \( (\psi = 78.46^\circ, \hat{\omega} = 0.3) \), (b) an inclined magnetic field at high frequency \( (\psi = 78.46^\circ, \hat{\omega} = 3) \), (c) a perpendicular magnetic field at low frequency \( (\psi = 0^\circ, \hat{\omega} = 0.3) \), and (d) a perpendicular magnetic field at high frequency \( (\psi = 0^\circ, \hat{\omega} = 3) \). The X-axis represents the inclination for the sputtered particle from the surface \( \Theta \) (with \( \Theta = 90^\circ \) represents a particle being sputtered in the direction perpendicular to the surface) and the Y-axis representing the energy at which the particle is sputtered from the wall. While the distribution along the X-axis his is subject to changes under different ion impact angle distributions, the distribution of the sputtered particles in the energy domain is a function of the surface energy and properties and independent of the ion impact angle distribution.

The strong role that the Hall force and \( E \times B \) drift play in dictating the ion impact trajectories leads to the ions impacting the wall at oblique angles causing particles to be sputtered from the surface in oblique trajectories. Fig. 3.4 (top left) shows the case with an inclined magnetic field at low frequency \( (\psi = 78.46^\circ, \hat{\omega} = 0.3) \) when the Hall force and the \( E \times B \) drift have a peak contribution creating a clear shift from perpendicular sputtering and a change in the distribution shape with particles being sputtered preferentially at a sputtering angle of \( \Theta \approx 60^\circ \). This is consistent with the ion impact angle distribution (seen in Fig. 3.3 and discussed in section 3.4) that is centered at an impact angle of \( \theta \approx 60^\circ \) at the time \( \omega t = \pi \).

As the wave frequency increases, the effect of the Hall force decreases, and at high frequencies \( (\psi = 78.46^\circ, \hat{\omega} = 3) \) the sputtering of surface particles is only affected by the \( E \times B \) drift. The lack of Hall force effects means that the ions impact the surface at more perpendicular angles causing the surface particles sputtering to be inclined towards perpendicular directions. The resulting change in sputtered energy-angle distribution (visible in Fig. 3.4 (top right)) is a slight displacement from a perpendicular sputtering distribution center.

As the magnetic field angle decreases the effect of the \( E \times B \) drift drastically decreases.
While the Hall force effect still plays a role in perpendicular magnetic fields at low frequencies (Fig. 3.4 (bottom left)) the particles are still sputtered with perpendicular inclinations. As a consequence of the weak dependence of the sputtered energy angle distribution on the impact angle distribution, both the $E \times B$ drift and the Hall force are needed to create a significant change in the ion impact angle distribution that translates into visible deviation in the sputtered energy angle distribution. When the wave frequency increases and the magnetic field has a perpendicular contact angle respect to the surface, both the Hall force and the $E \times B$ drift diminish leading to the electric field force dominating the ion trajectories and causing the ion to impact the surface at perpendicular angles. In the absence of competing forces the particle are sputtered preferentially in the perpendicular direction to the surface. The sputtered energy angle distribution center visible in Fig. 3.4 (bottom right) is centered around $\theta \approx 90^\circ$ that represents perpendicular sputtering of surface particles.

### 3.6 Flux propagation

The total flux of particles sputtered from the surface that propagates upstream is highly relevant in fusion applications since the interactions between the plasma core and the impurity particles gives raise to plasma instabilities during operation. The extent of these interactions are governed by the level of impurity flux that reaches the SOL from the FS wall. Changes in impurity flux levels have dramatic effects on the core operation due to the nonlinear dependence of the plasma core resistance on the contamination levels. Containing the impurity flux sputtered from the FS wall results in avoiding the collapse of the plasma core due to contamination.

Fig. 3.5 shows the effects of the sputtering yield perturbation on the impurity flux reaching upstream in different physical regimes. The figure shows heavy dependence of the magnitude of sputtered impurity flux on the wave frequency $\hat{\omega}$. When ICRH antenna is operated in high wave frequency conditions ($\hat{\omega} = 9$) (Fig. 3.5 (top)), the sputtered flux from the wall
Energy-Angle Distribution of Sputtered Impurities ($\omega t = \pi$)

$\psi = 78.46^o, \hat{\omega} = 0.3$

$\psi = 0^o, \hat{\omega} = 0.3$

$\psi = 78.46^o, \hat{\omega} = 3$

$\psi = 0^o, \hat{\omega} = 3$

Figure 3.4: Sputtered impurity energy-angle distribution for the case $\hat{\omega}_{ci} = 0.1 (\omega_{pi}), \hat{V}_{pp} = 200 (T_e)$ at time $\omega t = \pi$. Top left case a ($\psi = 78.46^o, \hat{\omega} = 0.3$), Top right case b ($\psi = 78.46^o, \hat{\omega} = 3$), Bottom left case c ($\psi = 0^o, \hat{\omega} = 0.3$), Bottom right case d ($\psi = 0^o, \hat{\omega} = 3$)
reaches \( \approx 2 \times 10^{20} \text{m}^{-2}\text{s}^{-1} \). As a consequence of the sputtering yield not experiencing major perturbations at high wave frequencies, the sputtered flux remains fairly stable throughout the sheath taking up to \( \sim 150 \) RF cycles to reach the upstream plasma. As the wave frequency decreases, the sputtering yield starts to experience oscillations during the RF cycles (Discussed in Sec. 3.3). When the wave frequency is of the order of the plasma frequency (Fig. 3.5 (middle)) \( \tilde{\omega} \approx 1 \) (regime of relevance for ITER operation) the changing sputtering yield causes the magnitude of sputtered flux from the wall to experience oscillations during the RF cycles. However, the background impurity level throughout the sheath changes at slower pace causing the oscillations to decay along the sheath. The oscillatory behavior is quickly damped out within the first 10 \( \lambda_D \) of the sheath from the wall.

When the wave frequency drops to values lower than the ion plasma frequency (\( \tilde{\omega} = 0.3 \)) (Fig. 3.5 (bottom)) dramatic perturbations in the flux of sputtered particles from the wall during a RF cycle appear. At low wave frequencies the ion impact energies fall in a region where the sputtering yield exhibits highly nonlinear changes with the sputtering yield even approaching 0 (\( Y_i \approx 0 \)) during certain segments of the RF cycle as discussed in Sec. 3.3. However, the dramatic perturbations in flux of sputtered particles from the wall happens over a larger time period as RF cycles are slower. This gives the background impurities more time to follow the change in sputtered impurity flux from the wall allowing the background impurity level to decrease several orders of magnitude during periods of low sputtering yield. The decrease in background impurity levels when operating under different wave frequency conditions is due to decrease of the density of the background sputtered particles. Sputtered particles propagation velocity is determined by the sputtering surface temperature and bonding potential, not by the RF sheath regime. As a consequence, impurities are sputtered with semi-constant energy distributions. The variation in sputtered impurity density is the dominant cause that leads to the changes in flux of sputtered particles from the wall.
Figure 3.5: Impurity flux levels at times $\omega t = \pi/2, \pi, 3\pi/4$ for varying $\omega$ for the case $\psi = 0^\circ, \dot{\omega}_c = 0.1 (\omega_{pi}), \dot{V}_{pp} = 200 (T_e)$ for Be FS wall at $\hat{x} = 0$. Top $\omega = 9\omega_{pi}$, Middle $\omega = 1\omega_{pi}$, Bottom $\omega = 0.3\omega_{pi}$.
### 3.7 Average Sputtered flux

The mean sputtered flux over one RF cycle ($\Gamma_{\text{avg}}$) quantifies the effective effect that the instantaneous flux of sputtered particles has on plasma core. The instantaneous flux of sputtered particles from the FS wall experiencing large perturbations during a RF cycle. As a consequence of these perturbations being damped out through the DS the level of contamination in the plasma core effectively sees a continuous source of impurity flux that is quantified by the mean sputtered flux that reaches the upstream plasma over one RF cycle provides. The mean sputtered flux over one RF cycle ($\Gamma_{\text{avg}}$) exhibits a heavy nonlinear depends on the operation parameters (magnetic field angle $\psi$ and normalized wave frequency $\hat{\omega}$).

Fig. 3.6 shows the behavior of the mean flux of sputtered particles $\Gamma_{\text{avg}}$ vs the wave frequency $\hat{\omega}$ for different magnetic field angles $\psi$. The figure shows variation in response of the mean flux of sputtered particles $\Gamma_{\text{avg}}$ to changes in wave frequency $\hat{\omega}$ in different wave frequency ranges: Low wave frequency range ($\hat{\omega} < 10$) (left figure), and high wave frequency range ($\hat{\omega} \geq 10$) (right figure).

As the wave frequency $\hat{\omega}$ approaches 0 (highly mobile ions), the mean flux of sputtered particles $\Gamma_{\text{avg}}$ converges and becomes independent of the wave frequency (Visible in Fig 3.6 (left)). The ion inertia delays the ion response to the changing RF voltage. As the wave frequency decreases, the variation in RF voltage happens at a significantly slower pace leading to the impacting ions becoming highly mobile in response to changes in RF voltages. There exists a certain threshold $\hat{\omega}$ at which the ions hit peak mobility and respond instantaneously to any changes in RF voltage that the ion inertia no longer plays a role and the ion impact energy becomes independent of the wave frequency. As a consequence of the dependence of the mean flux of sputtered particles $\Gamma_{\text{avg}}$ on the ion impact energy, the mean flux of sputtered particles $\Gamma_{\text{avg}}$ are also no longer a function of wave frequency $\hat{\omega}$. It is important to note that the threshold $\hat{\omega}$ is dependent on the magnetic field angles $\psi$, with higher $\psi$ having higher
thresholds.

As the wave frequency increases above the threshold wave frequency $\hat{\omega}$, the mean sputtered particle flux $\Gamma_{avg}$ increases linearly with increasing wave frequency $\hat{\omega}$ or decreasing magnetic field angles $\psi$. The increase in mean flux of sputtered particles $\Gamma_{avg}$ can be attributed to the increase in average sputtering yield (Discussed in Sec. 3.3) combined with the effect increasing average impact ion density ($n_i$). The average impact ion density $n_i$ increases rapidly with the initial increase in $\hat{\omega}$ reaching $n_i \approx 0.7 n_L$ at $\hat{\omega} \approx 200$. The rapid increase in average impact ion density $n_i$ overshadows the initial decrease in average normal impact velocity ($u_{xi}$). The linear dependence of mean flux of sputtered particles $\Gamma_{avg}$ on the wave frequency continues well into the high wave frequency range ($\hat{\omega} \geq 10$), until it peaks at $\hat{\omega} \approx 200$. Above $\hat{\omega} \approx 200$, the rate of increase in $n_i$ decreases until $n_i$ reaches the plateau $n_i=n_L$. The decrease in average normal impact velocity ($u_{xi}$) then dominates above $\hat{\omega} \approx 200$ leading to a sharp decrease in mean flux of sputtered particles $\Gamma_{avg}$. The average normal impact velocity ($u_{xi}$) converges at a wave frequency of $\hat{\omega} \approx 400$. The mean flux of sputtered particles $\Gamma_{avg}$ reaches a plateau value at $\hat{\omega} \approx 400$ as well (Visible in Fig 3.6 (right)). Our theory explaining the decrease in normal impact velocity $u_{xi}$ is the that at extremely low ion mobilities (high wave frequencies $\hat{\omega} \approx 400$), the potential drop changes at such a rapid rate that the ions do not get to time to react to an enhanced potential drop. This is supported by the convergence value of impact $u_{xi} \approx 4 \sim 5c_s$ being close to what is expected in classical sheaths without a RF enhanced potential drop.
Figure 3.6: Mean Sputtered Flux over a RF cycle from the Be FS wall for case \( \hat{\omega}_{ci} = 1 (\omega_{pi}) , \hat{V}_{pp} = 20 (T_e) \) for varying magnetic field angle \( \psi \). Top high ion mobility case \( (\omega \leqslant 10) \), Bottom \( (\omega \geq 10) \).
Chapter 4
Discussion and Conclusion

4.1 Discussion

We performed simulations ameliorating the impurity production at ICRH antenna in ITER and compared them to experimental data available in the literature [19, 20]. The simulations were performed for a deuterium plasma in an inclined magnetic field with a wave frequency equal to the plasma frequency ($\psi = 78.46^\circ, \hat{\omega} = 1$). The simulation was run for 45 RF cycles to ensure convergence to a periodic state. The average sputtered flux over one RF cycle was found to be $\Gamma_{avg} = 5.34 \times 10^{19} m^{-2} s^{-1}$. Taking the FS wall material to be Be (as proposed for ITER FS wall material [19, 20]) the mean flux of sputtered particles $\Gamma_{avg}$ translates into an erosion rate of $43 \text{nm/s}$. Most experimental data report the erosion rate from a fusion experiment rather than the mean flux of sputtered particles $\Gamma_{avg}$ as it is simpler to calculate. Since most published experimental data look at the broader image of erosion rate in a fusion experiment, they fail to report the operational parameters (the magnetic field angle $\psi$, and the normalized wave frequency $\hat{\omega}$) of the experiment. Comparing simulated data with the available experimental data without matching the magnetic field angle simulated should be an order of magnitude and qualitative comparison at best. Nonetheless we found that the simulated average flux to be in the same order of magnitude to experimental results from previous experiments ($\Gamma_{avg} = 11.9 \times 10^{19} m^{-2} s^{-1}$) performed on JET with Be FS antenna PFC and found in Bureš et al. [36]. We also found that the calculated erosion rate was almost twice of what was estimated in Wukitch et al. [21] ($15 - 20 \text{nm s}^{-1}$) with a B FS wall. It is important to note that the erosion rate was calculated for B instead of Be in Wukitch et al.
and the estimate of average flux found in Bureš et al. [36] assumes several operational parameters (Power delivered, Plasma density, FS wall effective area). Our simulated results lie in between the two experimental results. Taking this into consideration the numerical results can still be found to be in good agreement with experimental expectations.

Having such an erosion rate would mean that a 1 cm thick Be FS screen material would be eroded in \( \approx 2.3 \times 10^5 \) s. Any low Z FS material is expected to have a similar erosion rate and be completely eroded in a relatively short operation time in the vicinity of RF sheaths. This drastic restriction greatly limits the lifetime of these PFC. Assuming a discharge would take \( \sim 400 \) seconds, the RF antenna would need to be replaced after every 475 discharges. A non sustainable rate of operation for a material in a commercial reactor. The effect of the sputtered impurities on the stability of the plasma core, cannot be estimated from the current results as that requires several other simulation components. The erosion rate simulated was the gross erosion rate without factoring in self-sputtering by the impurities or redeposition that could lead to an enhanced erosion rate. In order to obtain the net erosion rate a global impurity transport code that would traces the sputtered particles paths until they are redeposited would be needed. Such a particle tracer would need to cover a range of plasma regimes (Debye sheath, Magnetic pre-sheath, Collisional Sheath upstream plasma) each with their different physical characteristic and time scales. Although such a simulation code would achieve more accurate numerical results, the computational cost, development time, applicability and feasibility greatly hinders the motivation for its development. Since the current code has already achieved numerical results with good agreement in comparison with experimental results, it can be used as a simulation tool for more accurate cases related to ITER antenna operation with trust in the simulated results.
4.2 Conclusion

In summary, we presented a new one-dimensional model based on previous work by Myra and D’Ippolito [28] describing the physical phenomena of enhanced sputtering yield from the FS PFC due to the interaction between the PFC and the RF sheaths. The model successfully captured the structure of the sheath, including the DS and the MPS, and their dependence on the different parameters \((\psi, \hat{\omega}, \hat{\omega}_{ci}, \hat{V}_{pp})\). The voltage rectification in the sheath, the ion and electron distributions, and the Sputtered impurity distributions were also successfully captured. The model has shown that the ion impact energy-angle distribution is heavily influenced by the regime of operation controlled by \(\psi, \hat{\omega}, \hat{\omega}_{ci}, \) and \(\hat{V}_{pp}\). In regimes of high magnetic field inclinations \(\psi = 78.46^\circ\) low wave frequencies \(\hat{\omega} = 0.3\), the incoming ions achieve highly oblique impact angles at \(\omega t = \pi\) with a part of the distributions avoiding impact and causing a back flow of ion flux. The ion distributions shift back towards perpendicular impact angles during periods of high potential drop. As the magnetic field angle \(\psi\) decreases and the wave frequency \(\hat{\omega}\) increases, the ion impact angle distribution shifts towards a perpendicular impact angle for larger portions of the RF cycle until they reach a semi-constant impact energy-angle distribution throughout the RF cycle.

Through coupling with F-Tridyn, the effect of the changing ion impact energy-angle distributions on the mean flux of sputtered impurities over one RF cycle \(\Gamma_{\text{avg}}\) was shown in Sec. 3.7. The mean flux of sputtered impurities \(\Gamma_{\text{avg}}\) was found to exhibit different responses to changing wave frequency in different wave frequency ranges. The erosion rate was calculated for ITER-like regimes, and was found to be \(\approx 43\text{nm/s}\). After comparing with experimental erosion rates and mean flux of sputtered impurities \(\Gamma_{\text{avg}}\), we concluded that the numerical simulations have shown good agreement with experimental results providing bases for the motivation behind the possible usage of the code as a reduced-parameter tool in Full-Device modeling.
4.3 Future Work

The current model has proven to have a robust ability in simulating RF sheaths including erosion rates and detailed sputtering physical features but the validation of the model is required to establish a trust in its simulation capabilities. Due to the dependence of the erosion rate on several parameters that are regularly unreported in literature such as magnetic field angle $\psi$, a dedicated collaboration on an active erosion experiment would ease the process of experimental data acquisition.

The best path forward to such a collaboration would be performing the experiment on a linear plasma device using a single strap antenna as a RF wave source. The use of a linear plasma device guarantees more control on the creation of far-field sheaths by placing an erosion target downstream on the opposite end of the electrically biased RF antenna. The use of a single strap antenna allows us to study large edge interactions without the need for large RF power levels. Single strap antennas are also easier to set up and rotate for changes in alignment. This allows us to study the effects of magnetic field misalignment on the erosion rate and sheath rectification physics. Validation data needed would not require specialized equipment as a simple measurement of the eroded thickness of the erosion target and the total RF operation time would be sufficient for the calculation of the erosion rate. The erosion rate is a quantity that can be simulated given the known operating conditions and hence easily verified with experimental data.

In addition to establishing trust in the models capabilities the following improvements can be made to enhance the usage of the model:

- Addition of impurity self-sputtering capabilities that has been shown to be a major concern with Carbon FS material.

- Expansion of the F-Tridyn lookup table data base to include larger sets of relevant materials such as Ni, Ti, W, Mo.
• Further investigations into the observed backward ion flux seen under restricted conditions in chapter 3.

• Effect of ion induced mixing between the Be coating and the Copper layer in the RF antenna on the lifetime of the ICRF device.
References


