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Measurement and Simulation of Deuterium Balmer-Alpha Emission from First-Orbit Fast Ions and the Application to Neutral Density and General Fast-Ion Loss Detection in the DIII-D Tokamak

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Measurement and Simulation of Deuterium Balmer-Alpha Emission from First-Orbit Fast Ions and the Application to Neutral Density and General Fast-Ion Loss Detection in the DIII-D Tokamak

DISSERTATION

submitted in partial satisfaction of the requirements for the degree of

DOCTOR OF PHILOSOPHY

in Physics

by

Nathan Glynn Bolte

Dissertation Committee:
Professor William Heidbrink, Chair
Professor Zhihong Lin
Professor Roger McWilliams

2015
DEDICATION

To my wife, Tamara, for making this possible.
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CURRICULUM VITAE

Nathan Glynn Bolte

EDUCATION

Doctor of Philosophy in Physics 2015
University of California, Irvine

Master of Science in Physics 2010
University of California, Irvine

Bachelor of Science in Physics 2001
University of California, Irvine

Bachelor of Science in Chemistry 2001
University of California, Irvine

RESEARCH EXPERIENCE

Junior Scientist 2008–Present
Tri Alpha Energy, Inc.
Rancho Santa Margarita, California

Laboratory Assistant 1999–2003
Tri Alpha Energy, Inc.
Rancho Santa Margarita, California

Laboratory Assistant 1998–1999
University of California, Irvine
Irvine, California

Laboratory Assistant 1997–1998
Brookhaven National Laboratory
Upton, New York

TEACHING EXPERIENCE

Teaching Assistant 2013
University of California, Irvine
Irvine, California

Math Teacher 2004
St. Margaret’s Episcopal School
San Juan Capistrano, California

Math, Physics, Chemistry Tutor 2003–2008
Bolte Tutoring Services
Laguna Niguel, California
SELECTED HONORS AND AWARDS

Undergraduate Research Fellowship 2000
National Science Foundation

President’s Undergraduate Fellowship 2000–2001
University of California, Irvine

PUBLICATIONS

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Generation and Transport of a Low Energy Intense Ion Beam

Recent results from the low inductance Z-discharge metal vapor ion source
N. DeBolt, A. Hershcovitch, B. M. Johnstona, N. Rostker, A. Van Drie, and F. Wessel
Measurement and Simulation of Deuterium Balmer-Alpha Emission from First-Orbit Fast Ions and the Application to Neutral Density and General Fast-Ion Loss Detection in the DIII-D Tokamak

By

Nathan Glynn Bolte

Doctor of Philosophy in Physics

University of California, Irvine, 2015

Professor William Heidbrink, Chair

Spectra of the Balmer-alpha radiation of first-orbit fast ions after charge exchange with edge neutrals have been measured in the DIII-D tokamak. Several collimated optics systems view the edge region—while avoiding any active beams—and carry light to a spectrometer tuned to the region of the 656.1 nm deuterium-alpha line. Viewing geometry and the high energy of the lost ions produce Doppler shifts, which effectively separate the fast-ion contributions from the bright, cold edge light. Modulation of the fast-ion source allows for time-evolving background subtraction. A model has been developed for the spectra of these first-orbit fast ions. The passive fast-ion D-alpha simulation (P-FIDAsim) is a forward model consisting of an experimentally-validated beam model, an ion orbit-following code, a collisional-radiative model, and a synthetic spectrometer. Eighty-six experimental spectra were obtained using 6 different neutral beam fast-ion sources and 13 different viewing chords. Parameters such as plasma current, toroidal field, electron density, plasma cross-sectional shape, and number of x-points were varied. Uncalibrated experimental spectra have an overall Spearman rank correlation coefficient with the shape of simulated spectra of 0.58 with subsets of cases rising to a correlation of 0.80. A single set of calibrated spectra (shot xvi
was measured and is used to estimate the neutral density throughout the cross-section of the tokamak. This is done by inverting the simulated spectra in order to find the best neutral density (in a least squares sense) required to best match the experimental spectra. The resulting 2D neutral density shows the expected increase toward each x-point. The average neutral density is found to be $3.3 \times 10^5 \text{cm}^{-3}$ at the magnetic axis, $2.3 \times 10^8 \text{cm}^{-3}$ in the core, $8.1 \times 10^9 \text{cm}^{-3}$ at the plasma boundary, and $1.1 \times 10^{11} \text{cm}^{-3}$ near the wall. A technique is developed which—after using first-orbit light to calibrate the system—can quantify losses from a wider variety of mechanisms. Fast-ion losses resulting from sawtooth crashes (shot 149941) is estimated to eject 1.2% of the fast-ion inventory, in good agreement with a 1.7% loss estimate made by the TRANSP code.
Chapter 1

Introduction

The human population of the world is projected by the United Nations to reach 9.6 billion by the year 2050 [8]. World energy consumption is projected to increase by 56 percent between 2010 and 2040 [9]. With petroleum expected to be consumed by the year 2100 [10] and considering the well-known effects of burning such fuels on climate, health, and environmental systems [11], it is clear that innovative energy sources need to be developed. One such potential source of energy is fusion.

Fusion is hoped by many to become an energy source for a world bursting at its seams. Fusion reactors have yet to produce any net energy though. Confinement and sustainment have proven to be very difficult and elusive problems indeed. However, research in the area of this yet-to-be-developed method of energy production may be time very well spent when one considers the upside of its success. For example, unlike fossil fuels, fusion would make no emissions into the atmosphere. Unlike fission, it would produce no long-lasting radioactive waste. And unlike several other forms of clean and renewable energy, fusion would have a high, constant output independent of weather or other external conditions. Heavy hydrogen, called deuterium, is found
in water and could be used as fuel in future fusion reactors. The theoretical energy yields of fusion are enormous with the deuterium extracted from one liter of water producing as much energy as burning 300 liters of gasoline [12]. Deuterium is so abundant, in fact, that these theoretical yields project a 2-billion-year supply in the form of ocean water.

1.1 Fusion Energy Research

Fusion is a reaction in which elements are combined to make heavier elements. It is the process by which stars “burn” and produce the wide array of elements. The most powerful of nuclear weapons, the hydrogen bomb, owes its strength to fusion.

Nuclei have to be moving so fast to overcome their natural electrostatic repulsion and fuse that temperatures of 100 million degrees are required [13]. At these temperatures (and well below), there is too much kinetic energy for electrons to stay bound to nuclei. Hot, unbound electrons and nuclei make up a state of matter called plasma. Plasma is a very unique state of matter, which not only acts as a gas or fluid but is also sensitive to electric and magnetic forces.

The charged nature of plasma means that it cannot touch a wall or solid object without neutralizing or cooling down. Thus, plasma must be positioned and controlled carefully within evacuated, hollow chambers. The energy of plasma and fusion products must be confined to allow energy to be recycled, keeping the reaction going. These are the basic reasons why confinement and control are such crucial aspects of fusion research.

While stars are formed by gravitational forces coalescing gas in space and compacting it until fusion results, here on earth, we take advantage of plasma’s charged nature to
use electric and magnetic forces to heat and confine the fuel. This method of fusion research is called magnetic confinement. One type of magnetic confinement device is the tokamak.

1.2 The Tokamak

Tokamaks are magnetic confinement devices that have doughnut-shaped (torus) chambers and helically-shaped magnetic fields. They were invented in the 1950s by Soviet physicists Igor Tamm and Andrei Sakharov [14]. By ramping up a large current through the center of the tokamak (the center coils in Figure 1.1), much like a transformer, wherein the plasma acts as the secondary winding, a toroidal electric field is created that drives a plasma current through the torus. The main toroidal magnetic field (around the larger radius) is produced by coils placed tightly again the vessel (shown in Figure 1.1). While there are coils to produce and shape the poloidal field (around the smaller radius), the induced plasma current itself produces much of the poloidal field. The sum of the toroidal and poloidal fields is what gives the net magnetic field its helical shape.

The method of driving current through the center of the tokamak (using a “center stack”) is a method of formation called “inductive” formation. Plasma current induced in this manner causes heating referred to as “ohmic” heating. Other methods of formation are called “non-inductive” formation and involve the use of neutral beams and radio-frequency (RF) heating to drive plasma current and produce the equilibrium fields shown in Figure 1.1.
1.3 The DIII-D Tokamak

The work presented in this thesis was carried out at the DIII-D tokamak at General Atomics in San Diego, California. The DIII-D tokamak has a roughly “D-shaped” cross-section, a major radius of $R_0 = 1.66m$, a minor radius of $a = 0.66m$, and a chamber elongation of 2.1 (see Figure 1.2). The toroidal field can vary from 0.5 to 2.2 T at $R_0$ while the toroidal plasma current has a maximum of 2.5 MA. The electron temperatures of up to 6 keV and ion temperatures of up to 17 keV cannot be achieved by ohmic heating alone. Eight neutral beams inject deuterium tangentially at up to 81 keV for a total of 21 MW of heating and current drive (see Figure 1.3). A 110 GHz electron cyclotron heating (ECH) system provides 6 MW of heating and off-axis current drive. A fast-wave (FW) system at 30 to 120 MHz gives 6 MW of current-drive and heating in the core.

DIII-D is a well-diagnosed experiment, which makes it a great candidate not only for doctoral work but for reactor-relevant conditions. Much of the work done today is designed to further the physics knowledge required for the design of the new International Thermonuclear Experimental Reactor (ITER).

1.4 The Importance of Fast Ions

In plasmas, there are different ways to classify ions. By species: there are fuel ions (deuterium and tritium), fusion products (helium and tritium), and impurities (mostly carbon in DIII-D). By energy: thermal ions ($\sim 15$ keV) and fast ions ($\sim 80$ keV - $\sim 2$ MeV). Fast ions are produced by neutral beam injection, RF heating, and fusion and are part of a larger class referred to as “energetic particles”. Fast ions are an important class of particles and are the main focus of this doctoral work.
Fast ions have larger orbits and gyro-radii than thermal particles, which gives them unique characteristics [15]. While fast ions contribute heavily to fusion rates (due to their high velocities), their role in plasma stability is far more complex and the focus of much on-going research. Fast ions, for example, can have a stabilizing effect by suppressing the internal “sawtooth” instability [16] or they can excite the $m = 1$ “fishbone” instability [17].

The study of energetic particles is a rich field both experimentally and theoretically. Diagnostics, for example, track fast-particle effects on fusion rates, plasma stability, and transport. Fast-ion confinement is crucial for energy recycling, fusion rates, and plasma stabilization. A sudden loss of fast ions would not only jeopardize plasma performance, but could also (especially in near-reactor conditions) seriously damage the inner (“first”) wall of the vessel. With an eye toward these concerns, this thesis will focus on a novel light detection diagnostic/simulation pairing aimed at the detection and quantification of fast-ion losses.

### 1.5 Existing Fast-Ion Loss Diagnostics

Fast-ion losses can be detected by a wide array of diagnostics. Simple foils and Langmuir probes to more sophisticated scintillators and neutral particle analyzers can detect particles [18] while radiation can be detected by looking at ion cyclotron emission (ICE) [18] or by leveraging existing visible light diagnostics like beam-emission spectroscopy (BES) [19].

The Beam-ion loss detector (BILD) at DIII-D [20] consists of two Faraday-cup-like particle detectors at the midplane ($z=0$): one an “active” channel detecting particles and the other blinded by an insulator to measure background noise. The viewing
angle allows only gyrating ions, not neutrals, to be detected. The BILD detects prompt losses from each beam, losses from instabilities, as well as enhanced losses during ion cyclotron heating. The relatively large collimating hole causes poor pitch- and gyro-angle resolution and ions below 10 keV cannot be detected.

The Fast-ion loss detector (FILD) at DIII-D uses a camera to image light made by fast ions as they penetrate a two-dimensional scintillator [21]. By doing so, it resolves the pitch angle and gyro-radius of the ions. The relatively low image capture rate of the camera (≤160 Hz) limits the frequency response of the FILD. However, portions of the phase space are integrated and measured at high frequency (1 MHz) using photomultiplier tubes (PMTs). A resolution of 1.4 cm has been achieved for the gyro-radius and 6° for the pitch angle. The FILD, along with reverse orbit following techniques, is being used successfully to study the affects on fast-ion loss rates during Alfvén eigenmodes and other MHD instabilities.

Solid state neutral particle analyzers (SSNPA s) at the National Spherical Torus Experiment (NSTX) [22] are silicon photodiodes that detect charge-exchange fast neutrals in the range of 30-100 keV. The output pulse height is proportional to the particle energy and therefore the particle energy distribution in this range is measured.

Langmuir probes measure edge electron density and temperature [23] and ion saturation current fluctuations due to fast-ion losses [18]. While a robust and relatively simple instrument, its major limitations are its very small spatial coverage and its inability to penetrate into the plasma core.

Ion cyclotron emission (ICE) is shown to be correlated with fast-ion losses from fishbones and other modes [15] [18] and amounts to qualitative detection of fast-ion losses.

Beam-emission spectroscopy (BES) is normally used to study light from injected neu-
tral beams. However, Heidbrink et al. noticed that BES channels also detect passive fast-ion deuterium-alpha (FIDA) light from interactions between fast-ions and edge neutrals [19]. Dedicated FIDA systems, such as the ones on MAST and the ASDEX Upgrade, have been shown to pick up large passive FIDA signals [24][25][26]. In these applications, the passive FIDA component is one of several sources of background radiation that must be subtracted to obtain the active FIDA signal. These observations of passive FIDA light are qualitative measurements of losses at best (they are, in fact, background nuisances) and therefore are the impetus for this doctoral work and for the development of a dedicated and quantitative fast-ion loss diagnostic by way of Doppler-shifted FIDA light.

1.6 A Novel Fast-Ion Loss Diagnostic

While the details of the experiments and simulation are in the following chapters, a quick introduction to the use of passive Fast-Ion Deuterium Alpha (passive FIDA) is helpful here. Fast ions that are expelled to the plasma edge (by any loss mechanism) produce bursts of fast-ion D-alpha (FIDA) light when they charge exchange with edge neutrals [19]. Presently, active FIDA diagnostics (at DIII-D, NSTX, ASDEX Upgrade, MAST, and other facilities [3][24]) use charge exchange with injected neutrals to diagnose confined fast ions. Similarly, passive FIDA measurements could take advantage of edge neutrals to diagnose fast-ion losses.

In a quantitative test of the technique, prompt losses from a modulated beam provide a known source of fast ions. The edge neutral density is measured by tomographic inversion of $D_\alpha$ and $D_\gamma$ emission. The FIDA spectrum is measured by an instrument that does not view the active beam. The sightlines are oriented in such a way as to Doppler-shift the light away from the cold background edge-light. The spectra
can then be compared with the predictions of a new passive FIDA simulation (P-FIDAsim) code that is based on the well-established active FIDA simulation code, FIDAsim [27].

Ultimately, the goal of passive FIDA is to detect and monitor fast-ion losses of any kind (prompt losses, instability ejecta, fusion products, etc.). However, before this could be done, a proof-of-concept needs to be performed using a controlled or known source of fast-ion losses. Neutral beam fast-ion prompt losses are the perfect candidate for such a known source of fast-ion losses. Knowing the prompt losses allows for the simulation of FIDA spectra and comparison with experimental measurements, both of which are the focus of this thesis.
Figure 1.1: Stripped down schematic of a tokamak showing poloidal and toroidal field coils but not the inductive formation coils [1].
Figure 1.2: The inside of the DIII-D tokamak [2]. Note the center-stack, various diagnostic and neutral beam ports, and the RF antennas. The walls are graphite.
Figure 1.3: The DIII-D neutral beam center-line geometry and naming scheme.
Chapter 2

Passive FIDA Diagnostic

This chapter discusses the physics and hardware concepts behind passive FIDA measurements, how experiments are carried out, and how the hardware is calibrated.

2.1 Diagnostic Concept

When fast ions enter the edge region of the tokamak (roughly anywhere outside the last closed flux surface (LCFS)) they enter a region of ever-increasing neutral gas density. Some ions subsequently undergo charge exchange with these edge neutrals. The result is a slow, cold ion (that will be ignored) and a fast neutral moving in a straight line in the direction it was last going as an ion. The fast neutral can be “born” in a variety of electron states. Whether born into an excited state or put into an excited state by subsequent collisions, a portion of fast neutrals is quickly in an excited state. Relaxation of these excited states is what produces photon radiation. In the case of FIDA, the transition of interest is from $n = 3$ to $n = 2$ (the so-called Balmer-alpha transition), which radiates at a resting wavelength of 656.1 nm.
Balmer-alpha radiation is commonly referred to as $\text{H}_\alpha$ radiation or, in the case of deuterium, $\text{D}_\alpha$. Figure 2.1 shows an introduction to FIDA emission in the case of a first-orbit fast-ion source.

Balmer-alpha radiation is red visible light and so is easy to detect. The light is picked up using collimating lenses and routed along fiber optics to a spectrometer where the light is dispersed by a diffraction grating. While the relatively cold edge region puts out high levels of light at the resting wavelength, the large velocity of DIII-D’s 80 keV fast ions gives a significant Doppler shift thereby separating out the fast-ion component from the thermal edge light. The Doppler shift is determined by the component of the fast ion’s velocity (at the time of emission, which is roughly the time of charge exchange) that is parallel to the line-of-sight of the detection chord.

### 2.2 Hardware

The work presented in this thesis utilizes two different sets of views and two different spectrometers.

One set of views is two “vertical” views designed originally to view beam $330^\circ$ left for use in active FIDA measurements [28] (see Figure 1.3 for the beam naming scheme and Figure 2.2 for the viewing geometry). These views have $f/4.4$ lenses (i.e. focal length 4.4x the diameter) mounted under the midplane and light is carried to the spectrometer via 1500 $\mu m$ fibers. The second set of views is eleven “oblique” views designed as an upgrade to the FIDA system to view beam $210^\circ$ right [29]. These eleven chords each have a bundle of three 1500 $\mu m$ fibers for greater light pickup.

Each of these views can go to one of several detectors by way of a patch panel. The majority of this work utilizes the original FIDA spectrometer [30]. This spectrometer
is a Czerny-Turner with $f/4$ lenses, an 1800 grooves/mm grating, and a 300 mm focal length. A $1 \times 2$ mm rectangular neutral density filter is placed at the focal plane to heavily reduce the bright, non-shifted signal near 656.1 nm which would otherwise saturate the camera. A charged-coupled device (CCD) camera (VelociCam VC105A from PixelVision) is used to detect the dispersed signal. The CCD chip is a $652 \times 488$-pixel ($8 \times 6 mm^2$) array with 1-ms integration time and is set up to image two views at once. The spectral range of this system ($\sim 648 - 664$ nm) allows the viewing of both red- and blue-shifted signals. Figure 2.3 shows a schematic of the spectrometer.

Unfortunately, toward the end of the campaign, the camera in the Czerny-Turner spectrometer stopped working, preventing a post-campaign calibration and forcing the use of a second spectrometer. This HoloSpec transmission grating spectrometer uses a Sarnoff CAM1M100 CCD camera to image six simultaneous spectra onto a $1024 \times 1024$-pixel chip [29]. To avoid the bright region near 656 nm, this system only images the blue region of $D_\alpha$ emission ($\sim 650 - 654$ nm).

### 2.3 Experimental Design

Several factors were taken into account to maximize the probability and amplitude of the fast-ion edge-light signals from beam prompt losses. The signals would be swamped by active emission if the chords were to view an active beam. Therefore, any beam that the chosen views cross is turned off for the duration of the discharge. The next issue is understanding which beams would produce prompt losses near the two edge regions in our lines-of-sight. Since fast ions in DIII-D have a mean-free-path corresponding to hundreds of toroidal transits, they can be considered single, collisionless particles and their trajectory inside the tokamak can be calculated by solving the Lorentz-force equation. By tracking ion orbits originating from various
points along a given beam, the region of greatest prompt losses is determined. In this manner, a modified version of the P-FIDA simulation (to be discussed below) determines which chords should be paired with which beam (and at what field and plasma current) to get the highest signal from prompt losses. In order to assure sufficient signal, the plasma current is often ramped up and then down over the course of the shot. This has the effect of sweeping the first-orbit region around the tokamak toroidally, giving a larger probability of passing through the detection volume.

Doppler shifting the fast-neutral D$_\alpha$ line is not sufficient to reveal the signal. The edge-region is filled with light in the D$_\alpha$ range and also contains lines from carbon, oxygen, and boron. This light comes from scattering, reflections, Bremsstrahlung, and radiation from the cold edge neutrals and needs to be removed to reveal the fast-ion component. Beam modulation provides this background signal as a function of time. Thus, the beam providing the prompt losses is modulated at 50 Hz at 50% duty cycle. Beam-off signals are then subtracted from adjacent-in-time beam-on signals. This process, often called “time-slice subtraction”, produces a “difference” spectrum, which is the portion of the spectrum resulting only from prompt losses.

## 2.4 Calibration

Two types of calibrations were performed for the HoloSpec spectrometer: spatial calibration and intensity calibration.

Each view has its own collimator which limits the volume sampled to a shallow cone with a nominal radius of 5 cm. Spatial calibration simply means finding the nominal radius as well as two points along the center-line of each chord that will then define that chord. The first point of each chord is its collimating lens or the mirror that
directs the view into the vessel. These locations are readily measured outside the vessel and do not change much over time. The second point defining a chord is measured inside the vessel. During a period when the tokamak is being ventilated (a “vent”), two scientists enter the vessel and set up a table with a paper target lying in the midplane \((z = 0)\) in the region of the chords. A third scientist then shines light into the fiber optic outside of the vessel. The back-filled light makes a spot on the target which is marked and its position is measured. In this manner, the location of each line of sight is determined.

Next is the intensity calibration which correlates the voltage out of the spectrometer to the spectral radiance of a source. Spectral radiance is a typical unit used in spectroscopy thanks to its very convenient quality of being conserved. This means that the spectral radiance of a source is equal to the spectral radiance on the detector \([31]\). Even though plasma emits light throughout its volume, the light is ultimately integrated onto a surface. This makes spectral radiance (the emission intensity of a surface) the natural unit of measure.

The calibration is performed using a calibrated, uniform light source (by Labsphere \([32]\)). Labspheres (or other such sources) are very useful thanks to two qualities they have: 1. they are Lambertian sources, which means their spectral radiance is independent of viewing angle (meaning the exact alignment during calibration is not important) and 2. they have a calibrated intensity as a function of wavelength. The Labsphere is an 8-inch sphere with a 2-inch hole in the side. Any view that is confined to this 2-inch hole has the same, known spectral radiance incident upon it. Therefore, the sphere is placed inside the vessel and positioned such that the entire cross-section of a back-filled view passes unobstructedly through the Labsphere opening. The back-fill light is then turned off while the Labsphere is turned on. The spectrometer is then triggered to capture data (that is, integrate the incoming light for a given period of
time, usually 1 ms). In this manner, the attenuation and effects of windows, lenses, fibers, couplers, the dispersion element, and the camera are all taken into account. A given voltage and integration time from the spectrometer can thus be converted into the spectral radiance of the source in units of, for example, $\text{ph}/\text{s} - \text{m}^2 - \text{sr} - \text{Å}$. This process is carried out for each of the views.
Fast Ion D-Alpha (FIDA): Balmer-alpha radiation from recently neutralized deuterium. $n: 3 \rightarrow 2$ (656.1 nm)

Figure 2.1: The basics of FIDA emission (using prompt losses as an example). Adapted from [3].
Figure 2.2: The viewing geometry and naming scheme for the vertical and oblique chords. (a) Elevation View: A cross-sectional view projecting all the way around the tokamak (i.e. including all toroidal locations). (b) Plan View: Looking down on the tokamak.
Neutral Beam Provides a Known Source of Fast-Ions

A Known Source of Fast Ions:

- Neutral Beam Species and Energy
- Plasma Profiles
- ADAS Beam-Stopping routines

Fast-Ion Birth Locations and Velocities

Collection Lens

Tokamak Neutral Density Filter Attenuates ~3 nm of spectrum near cold Dα line (656.1 nm)

1. Fast-Neutral Injection
2. Ionization
3. Translation Across Vessel
4. Charge-Exchange with Edge-Neutral
5. Born with / excited to n=3 state
6. Relaxation to n=2 (656.1 nm Photon)
7. Doppler-Shifted Light Collected

Ionization Radiation Spectrometer Simulated Signal Known prompt-losses + Known edge-neutral profiles = Known light source

Figure 2.3: Schematic of FIDA spectrometer. Adapted from [4].
Chapter 3

Experimental Data Analysis

This chapter discusses the time-slice subtraction method used to obtain the time-independent experimental spectra, how the quality of the signals is maximized by experimental design as well as post-experimental data analysis, and closes by discussing the uncertainty of the measurements.

3.1 Extraction of Fast-Ion Spectra

The raw spectra obtained from the spectrometer are 2D signals of CCD voltage versus pixel number as a function of time. The semi-raw contour plot in Figure 3.1 (where pixel has already been converted to wavelength) reveals several features. A neutral-density filter at the focal plane of the spectrometer blocks out most light in the region of 6550 to 6580 Å as can be seen by the black portions of the spectrum. However, the heavily-reduced $D_\alpha$ line can still be seen at 6561 Å. The band at 6500 Å is a strong oxygen V ($O^{4+}$) line.

Averaging Figure 3.1 over time gives Figure 3.2, which reveals more features. Impurity
Figure 3.1: Raw edge-light spectrum vs. time from shot 149954, channel F01, chord P6, using beam 30-left.
lines from boron, carbon, and oxygen are easily identified as is the residual D$_\alpha$ line. The region of the neutral-density filter is noted. The region between the OV line and the left side of the neutral-density filter is the region suspected of containing the fast-ion signal (based on a simple Doppler-shift calculation using the ion velocity and viewing geometry).

Figures 3.1 and 3.2 are only semi-raw as they have a wavelength baseline. The original basis is simply pixel number until a fiducial and the dispersion are calculated. This is done in the following manner. First, two well-identified and well-resolved lines (called fiducials) must be located. The two largest lines still having a Gaussian shape are the oxygen V line at 6500 Å and the D$_\alpha$ line at 6561 Å. These two well-known lines are used as fiducials to correlate the pixel number with wavelength. Gaussians are fit to both the D$_\alpha$ and the oxygen V line regions of the spectrum, giving the center pixel location for each line and the number of pixels between them. The difference in wavelength between these two lines divided by the difference in their pixel numbers gives the dispersion in Å/pixel. Each pixel position is then converted to its corresponding wavelength value by using the dispersion along with the position of one of the lines. This method assumes a uniform dispersion. However, the dispersion is, in general, a function of wavelength. The use of a uniform dispersion is justified by the narrow (∼150Å) wavelength range of the spectra (see Figure 3.3).

The region from about 6510 to 6540 Å in Figure 3.1 shows a clear, periodic variation in time and is at a wavelength consistent with the Doppler shifts expected from first-orbit fast ions and the viewing geometry. Taking a lineout plot of Figure 3.1 at 6530 Å gives Figure 3.4(a) where a clear periodicity can be seen and appears to be correlated with the neutral beam power (3.4(b)), which is the intended source of fast-ion losses. The zoomed-in plot (3.4(c)) (with the low-frequency components removed for clarity) makes a definitive correlation between the blue-shifted light and the beam power.
The desired fast-ion first-orbit component of Figure 3.1 is extracted thanks to the use of beam modulation and time-slice subtraction. The rise and fall of the spectral signal in Figure 3.4(c) is due to the increase and decrease of passive edge-light resulting from the modulation of the 30-left beam and its corresponding prompt losses. First, a time range is chosen over which to average the spectra. Then Figure 3.4(b) is used to determine the times during which the beam is on and the times during which the beam is off. The fast-ion spectrum is found by time-averaging the spectrum during all beam-on times (the black spectrum in Figure 3.5(a)) and subtracting from it the spectrum averaged over all beam-off times (the red spectrum in Figure 3.5(a)). The resulting difference, or “fast-ion”, spectrum is shown in Figure 3.5(b).

When a calibration is available, each pixel (or wavelength) is then multiplied by its calibration factor, which gives the final, calibrated spectrum in spectral radiance versus wavelength.
3.2 Signal Improvement

After developing a high-throughput optics system, there remain two areas left to optimize the spectral quality: experimental methods and data-analysis methods.

The data presented thus far already motivate the need to take every measure to optimize the fast-ion signal. The intensity of the fast-ion spectrum is proportional to the fast-ion first-orbit density, which is not very large. As can be seen in Figure 3.5(a) (representing a relatively large fast-ion signal), the fast-ion portion of the spectrum amounts to less than 10% of the raw spectrum in that region. The oxygen and carbon impurity lines are generally much larger than the blue-shifted region of the raw spectrum. This means that only small imperfections in the time-slice subtraction
Figure 3.4: (a) Lineout plot of Figure 3.1 at 6530 Å along with (b) beam power. (c) Zoomed-in portion of plots (a) and (b) with the DC component removed from the spectral lineout data illustrating the beam-correlated modulation of the passive FIDA signal.
Figure 3.5: Time-averaged spectra from Figure 3.1. (a) Time-averaged spectrum during beam-on times (black) and time-averaged spectrum during beam-off times (red). (b) Difference between beam-on and beam-off spectra, i.e. the fast-ion spectrum.
process can result in significant structures in the final, fast-ion spectrum. See, for example, the negative values in Figure 3.5(b) at 6586 Å due to imperfect carbon II subtraction.

Several aspects of the experimental design are focused on obtaining high-quality signals. Most fundamentally, the tokamak is run in a stationary manner (the so-called “L mode”) known to avoid edge-localized modes (ELMs) [33]. ELMs eject high-energy particles into the edge region, obscuring the first-orbit signals. Another area of focus is identifying the toroidal region of prompt-loss ejection. While P-FIDAsim suggests the region of greatest prompt losses, this is confirmed experimentally by ramping the plasma current up and down past the optimal value predicted by the simulation. Once a good plasma current is chosen, a shot is taken at that constant value to provide prompt losses over a longer period of time, improving the signal-to-noise ratio (SNR) of the time-averaged spectra.

The final way to improve the spectral quality is the post-processing of the signals. While several areas of data analysis were explored, it is found that the most important issue is instabilities. Even ELM-free plasmas can have instabilities that affect the edge region. The well-known sawtooth instability [16] occurs often in DIII-D plasmas and can, in principle, cause changes in edge plasma spectra. The black curve in Figure 3.6(a) is an electron cyclotron emission (ECE) trace showing the characteristic slow rise and fast fall of the sawtooth crash. Since the fast crash of this instability can possibly heat (Doppler broaden) the edge region or cause bulk motion (Doppler shift), data analysis codes were designed to identify these sawteeth and exclude the times near crashes from the time-averaging. The red dashed lines in Figure 3.6(a) show where the code identified sawtooth crashes. Figure 3.6(b) shows the difference between a spectrum that includes sawtooth crashes and one that does not. By removing the crash times, the fast-ion signal is larger, the signal has a more appropriate
baseline in the extreme wavelength regions (that is, it goes to zero), and the imperfect subtraction of the carbon II line is improved.

Figure 3.6: (a) Electron cyclotron emission for shot 149955. Red dashed lines mark where the code found sawtooth crashes. (b) Spectra for channel F01, chord P6 showing improved signal when removing times near sawtooth crashes. Beam 30-left is the source of fast ions.

### 3.3 Uncertainty and Signal-to-Noise Ratio

Uncertainty is created in the spectral signals due to photon statistics (low signal intensity), electronic noise, and possibly vibration of the optics (especially in the radial direction).
An estimate in this uncertainty is obtained by taking advantage of the time-dependent nature of the signals. The spectra shown in plots like Figures 3.2 and 3.5(a) are found, as discussed, by time-averaging over several seconds. The error is found prior to time-averaging by considering each pixel’s signal in turn as a function of time. The method used is essentially that of taking a mean (of values with uncertainties) and giving the standard deviation of the mean (Section 4.4 and Equation 4.14 of reference [34]).

The signal’s time resolution is first reduced by grouping together five adjacent beam-on (or beam-off) pulses. The mean of this group becomes a data-point while the standard deviation of the group is its uncertainty. In this way, thousands of points in time become about 100 points, all with their own uncertainties. Averaging these 100 points gives the mean for that pixel while the uncertainty of the mean is the average of the 100 uncertainties divided by the square-root of the number of points (100). This process is carried out for each pixel to obtain the beam-on time-independent spectra and then again (during the beam-off times) to obtain the beam-off time-independent spectra. An example of the result can be seen in Figure 3.7(a).

Since the fast-ion spectra come from the difference of the beam-on and beam-off spectra, standard error propagation is used to find the fast-ion spectral error (i.e. \( \sigma_{fast\_ion} = \sqrt{\sigma_{beam\_on}^2 + \sigma_{beam\_off}^2} \)). The results can be seen in Figure 3.7(b).

The signal-to-noise ratio \( (signal^2/\sigma^2) \) is about 30 at the peak of the fast-ion signal. While this is not a bad SNR, many other cases have much poorer SNR and therefore emphasize the need for careful hardware and experimental design as well as careful data analysis.
Figure 3.7: (a) Beam-on spectrum from Figure 3.5(a) showing the modest errors due to variations in time. (b) Fast-ion spectrum from Figure 3.5(b) showing the relative increase in the errors from the raw spectrum. For clarity, not all error bars are shown.
Chapter 4

Passive FIDA Simulation

The spectra of poorly-confined first-orbit ions charge-exchanging in the edge region lends itself well to forward modeling. Modeling this phenomenon acts as a quantitative test of the novel use of passive FIDA light to measure losses. The neutral beam acts as a well-known source of fast-ion losses and the signal depends linearly on the edge neutral density, allowing for the measurement of the neutral density. In addition, forward modeling enables the interpretation and quantification of other fast-ion losses such as the sawtooth instability. This chapter discusses the main components of the simulation, its successful verification, and its sensitivity to systematic variations in the neutral density and plasma profiles. Specific information on the code’s location, file names, and workflow can be found in Appendix A.

4.1 Code Structure

P-FIDAsim has six main parts: A beam model determines where ions originate when injected neutrals are ionized. An ion orbit-tracking and capture module calculates the
ion orbits and accumulates the portions of orbits that pass through the chosen lines of sight. A neutral density model calculates a normalized neutral density from plasma profiles. A module called “mesh” interpolates all pertinent values onto each captured ion location. The “atomic loop” portion of the code runs a collisional-radiative model to find the photon emission rates and wavelength shifts. And finally, the “spectra” module compiles and organizes the emission information into spectral intensity versus wavelength plots.

Figure 4.1: A basic description of the passive FIDA simulation.

4.1.1 Beam Model

The beam model calculates the ion birth locations and velocities for the chosen neutral beam (see Figure 4.2). A neutral beam is a beam of highly-energetic and highly-
directional deuterium gas. The injected neutral gas is mostly ionized by charge exchange with deuterium ions, but also by electron impact as well as charge exchange with non-fully stripped carbon impurities. The high-energy neutral gas has a probability of ionizing at any given location based on properties of the beam and the plasma. Looking at the phenomenon from the perspective of beam neutrals, the beam is said to “attenuate” as it enters the plasma, but this is really the “birth” of ions and the starting point for the simulation.

The beam model takes, as inputs, electron and carbon (the main impurity) density profiles, the electron temperature profile, the equilibrium fields, the beam energy, and the number of desired ion birth locations. The deuterium ion density is inferred from the electron and carbon densities by using quasi-neutrality (i.e. \( n_d = n_e - 6n_c \)). Realistic geometry and beam characteristics such as beam center-line, width, height, and divergence are gathered for the requested beam. Because neutrals move in a straight line, a Monte Carlo code selects many lines, or “rays”, as potential pathways for the neutrals. Together, all of the rays produce the desired degree of divergence as is known from measurements and is stored in the code. The beam attenuation profile is then calculated along each ray using the Atomic Data and Analysis Structure (ADAS) [35] beam-stopping routines. Monte Carlo selection is used to choose ionization locations along each ray. The beam attenuation rate at that location is then used to give an ion birth rate. Combining this list of birth rates with the desired number of ions gives a final list of ion birth locations and velocities. Any trajectories that intersect beam collimators are removed from the final output. Any neutrals that do not ionize are collected at the opposite wall and are given in the model’s output as “shinethrough”.

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4.1.2 Ion Capture

The ion capture module consists of calculating and tracking ion orbits and determining if and where each ion enters the volume of the chosen lines-of-sight. The main inputs for this code are the equilibrium fields and the ion birth locations and velocities from the beam model. Other inputs are chord names (to retrieve chord geometry), chord radius, ion orbit step-size, and total length of ion orbit (to determine the number of steps to take).

A collisionless condition is assumed and ion orbits are tracked from their birth location by differentially solving the Lorentz force equation: \( \vec{F} = q[\vec{E} + (\vec{v} \times \vec{B})] \). This is justified by the fact that confined fast ions in DIII-D make, on average, hundreds of toroidal orbits before colliding with another particle while first-orbit studies involve
only one or two orbits. The time integrator used is a predictor-corrector Adams-
Bashforth-Moulton differential equation solver [36].

The time it takes to calculate the ion orbits is what makes this the most intensive set
of calculations in the simulation. Each ion orbit contains a large amount of data and,
therefore, the code is designed to not save all of this unnecessary data. Instead, each
ion orbit is calculated one at a time and only the discrete steps that enter a desired
line-of-sight are saved. The remaining portion of the orbit is discarded. The output
of this module is a list of ion locations and velocities detected within the volume of
each chord.

4.1.3 Neutral Density Model

The neutral density model determines the functional form (in arbitrary units) of
neutral density resulting from the attenuation of neutrals launched from the walls
due to electron-impact ionization and charge exchange with deuterium. While other,
better, codes exist that calculate realistic neutral densities (in 2D or even 3D), these
codes require data that is not readily available here. This model is less complete
and far simpler by comparison, however, it utilizes all of the data we do know with
confidence: the 1D plasma profiles. Neutrals do not (for these purposes) respond to
magnetic and electric fields and there exist localized neutral sources and sinks. For
these reasons, neutral density is not generally a flux function. However, ionization of
neutrals takes place as a result of plasma ions and electrons which are flux functions.
Therefore, neutral density is assumed to be a flux function as an approximation
whenever further information is not available. It is hypothesized at this point that
the neutral density actually has a ρ and z dependence, with the latter coming from x-
points and divertors. For now, a uniform source is assumed to emanate from the walls
and the z-dependence will be determined later by scaling spectra up to experimental
values using the inversion method discussed in Section 6.1.1.

The 1D neutral density model begins by “launching” a neutral atom inwardly from the
wall with a nominal energy where it encounters the experimentally-determined elec-
tron and main-ion profiles. The motion of the neutral is along $\nabla \rho$ (i.e. perpendicular
to the magnetic field lines), and therefore the profiles are unchanged perpendicular to
the neutral’s line of motion, thus justifying the 1D nature of the model. Velocities are
chosen randomly in all three dimensions and the velocity is normalized to correspond
to the total energy of 3 eV (a typical energy after molecular dissociation). While
a velocity is generated in 3D, only the component along the 1D line is considered.
Thermal ions are launched repeatedly (also with random but thermal velocity). The
probability of charge exchange (CX) between the ions and the neutral, the probability
of ionization from electrons, and the neutral’s motion through the 1D cells along the
line of motion are all monitored. Charge exchange is interpreted as a new neutral
being “born” which is then given the velocity of the incoming ion. Ionization means
the neutral is lost and a new neutral is launched from the wall to start the process
over. If neither of these events take place before the time it would take the neutral to
pass to the next cell, then the neutral is moved to the next 1D cell where the tracking
process begins again. The neutral density is then proportional to the time spent in
each cell and is normalized by cell size, number of Monte Carlo particles, and an
arbitrary scaling factor (to keep the maximum value close to 1). Neutrals continue
to be sourced inward from the wall until a functional form is converged upon.

Next, the calculated neutral density could be converted from flux coordinates to physi-
cal (R,z) coordinates but instead the 1D model is used repeatedly (moving the source
position around the wall poloidally) to find the density for the entire (R,z) cross-
section of the tokamak. This is done for three reasons: 1. While the neutral density
model does assume a flux function, the coordinates are entered as physical 1D coordinates as are required to convert from velocity to time. As such, density values will not be the same for widely-varying field gradients because in some regions it takes longer for a neutral to pass from one flux surface to another compared to other regions. 2. Physical coordinates (R,z) are a natural choice as they are used for the captured ions. 3. Later experimental altering and scaling of the neutral density is necessarily done in (R,z) coordinates.

The challenge in using the 1D neutral density model repeatedly to give neutral density for the entire (R,z) cross-section of the tokamak is that each 1D run must be ever-perpendicular to the magnetic flux surfaces. This condition is met in the following manner. First, $\nabla \rho$ is calculated over the full (R,z) grid. A starting point at the wall is chosen. Defining the “path-vector” as the vector formed by two positions along the neutral’s path, a path inward is then chosen by minimizing the path-vector dotted into $\nabla \rho$. This creates a path that is most perpendicular to the field lines (i.e. heading “downhill” in a contour plot of $\rho$). The ray then stops if it begins to move uphill or if the path and $\nabla \rho$ diverge beyond acceptable limits. This process continues with each successive starting point progressing poloidally around the vessel wall. The process creates a relatively large and chaotic data set which is quiet redundant. Therefore, overlapping density values are averaged and the entire data set is interpolated onto a uniform 2D grid. The final step is to re-normalize the entire grid to a maximum value of 1 along the outboard wall. The result is a density flux-function expressed in terms of R and z (see Figure 4.3).

With x-points at the lower (and potentially upper) boundary, neutral density will likely have an elevation (z) dependence as well. However, the z-dependence is not accounted for here but rather comes from experiment and is the subject of section 6.1.
4.1.4 Mesh

The mesh module gathers the various profiles (density, temperature, etc.) and interpolates their values onto the specific ion locations determined in the ion-capture module.

This code is called “mesh” as a historical connection to FIDAsim where, at this point, a 3D grid (or “mesh”) would be set up in space and profiles would be interpolated onto this grid. While several grids could be set up in P-FIDAsim, each collinear to
a line-of-sight, it is more natural and efficient to use the discrete locations already
determined by ion capture. Several profiles are interpolated onto each ion location:
ion temperature, impurity density, electron density, electron temperature, and neutral
density. The deuteron density at each ion location is found by quasi-neutrality: \( n_D = n_e - 6n_c \), where \( n_c \) is the carbon density (the main impurity at DIII-D). The electron collision rate \( (n_e \langle \sigma v \rangle) \) is also found at each ion location. The fractional population of each atomic level (up to \( n = 4 \)) is determined for all neutrals assuming collisional-radiative equilibrium using local plasma parameters. Lastly, the equilibrium magnetic field is found at each ion location for later use in finding the Stark effect.

4.1.5 Atomic Loop

This portion of the simulation carries out the “atomic physics” calculations by running
a collisional-radiative model. In particular, it uses the charge-exchange probability
between promptly-lost fast ions and cold edge-neutrals, gives the subsequent photon
emission rates, and determines the Doppler and Stark shifts.

The probability that edge neutrals and fast ions charge exchange is a function of the
relative population of the quantum states of the neutrals, the relative velocity between
the ions and the neutrals, and the quantum states that the new, fast neutrals are
born into. Because edge neutrals are \( \sim 10 \text{ eV} \) while fast ions are \( \sim 80 \text{ keV} \), a great
simplification can be made by letting the relative velocity be the fast-ion velocity,
i.e. \( \vec{v}_{\text{rel}} = \vec{v}_{fi} - \vec{v}_n \approx \vec{v}_{fi} \). Edge neutrals are limited to the first four quantum states
as are the fast neutrals resulting from charge exchange. The reason for this is that
the occupation levels for \( n > 4 \) are very low in a collisional-radiative equilibrium.
This mean that the fraction of charge-exchange events that produce an \( n = 3 \) fast
neutral from an initially \( n = 5 \) cold neutral is negligible. The atomic loop code runs
a collisional radiative model, which considers intermediate atomic levels up to \( n = 7 \) and outputs the photon emission rate for the Balmer-alpha \( n = 3 \to 2 \) relaxation. Note that, while other transitions certainly exist and have their own photon emission rates, this simulation ignores those lines and only tracks \( D_\alpha \) light. The Doppler shift is then calculated by taking the dot product of the fast neutral’s velocity (i.e. that of the fast ion at the time of charge exchange) and the unit vector of the line-of-sight. This “local approximation” (that \( \vec{x}_{fast, ion} \approx \vec{x}_{cx, neutral} \)) is justified by the finding that the time between CX and emission is on the order of several nanoseconds. This means the distance traveled before emission is \( \lesssim 1cm \) (for comparison, the chord widths are \( \sim 10cm \)). This reduces the spatial accuracy of the simulation but is a great simplification over tracking each neutral until it radiates. The Stark effect further shifts the wavelength of light based on the electric field experienced by the fast neutral. The electrostatic component of the field is ignored as the effect is heavily dominated by the \( \vec{v} \times \vec{B} \) term. The Stark effect has unique probabilities for the photon to have nine different shifts. These probabilities are normalized to one so that, while the photons are binned into different wavelengths, their total number is conserved.

### 4.1.6 Spectra

The spectra section of the code takes the raw, unorganized spectral data from the atomic loop module and bins the photon counts together into wavelength bins while separating them according to which line-of-sight they are in.

### 4.1.7 Scaling

The final step is to provide appropriate scaling and units to the spectra.
At this point, the output (call it E) has the units of photons/sec and needs to be converted to more traditional spectral radiance unit of \( \text{photons/sec} - m^2 - sr - Å \). This is done (at least conceptually) by first finding the local emission rate per unit volume of neutrals and per solid angle of emission and then integrating those values along each line-of-sight. Since, to first order, the radiation is isotropic, photons are radiated into \( 4\pi \) Sr. Integrating along the LOS means adding up all individual emission rates per unit volume and multiplying by the length through each volume bin. With the emission volume being defined by the group of captured ions (i.e. the chord’s cross-sectional area (A) times the length along the LOS occupied by ions (\( \ell \))), this whole calculation simplifies such that the spectral radiance \( S = E\ell/(4\pi V \Delta \lambda) = E/(4\pi A \Delta \lambda) \), where \( \Delta \lambda \) is simply the wavelength bin size chosen by the spectra module.

The spectra still need to be scaled up to realistic values as they currently reflect the small number of simulation ions (typically 200,000) not the massive number of ions actually in the experiment. This final scaling factor comes from comparing an experimentally-measured value with a simulated one. The ratio of the experimental neutral beam current and the simulated neutral beam current is chosen for this purpose.

The experimental beam current \( (I_{exp}) \) is measured for each beam and shot number at DIII-D and is therefore easily retrieved. Because the beam current is measured near the output aperture, any neutrals that pass completely through the plasma, striking the opposite wall (called “shinethrough”) are included in the current measurement. This means that any calculation of simulated beam current must also include shinethrough. Experimental measurement of neutral beam current is essentially a measure of the neutral flux into the plasma chamber as if all neutrals were fully ionized.

The simulated beam current is not readily available and needs to be calculated. The
beam model, however, does not contain any neutrals, per se. It is a list of ion birth locations and no longer has any information about any beam neutrals. This means that the simulated beam current cannot be found simply by placing an imaginary Amperian loop somewhere around the beam. A method must be used which incorporates all beam ions as well as the shinethrough neutrals. These subtleties are satisfied simply by volume-averaging the beam current. Consider a cylinder of cross-section \( A \) enclosing the beam ions in Figure 4.2. The current, \( I_{\text{sim}} \), through the cylinder is \( JA \), where \( J \) is the current density. Deuterium neutral beams do not have a single energy, they have three: the full energy (80 keV, for example), the half energy (40 keV), and the one-third energy (\(~27\) keV). By including each of the three beam energies, the total beam current becomes

\[
I_{\text{sim}} = \frac{ZeN}{\ell} \sum f_i v_i
\]  

(4.1)

where the sum is over the three beam energies, \( Ze \) is the ionic charge, \( N = N_{\text{birth}} + N_{\text{shinethrough}} \), \( \ell \) is the length of the beam, \( f_i \) is the fraction of ions with the \( i^{\text{th}} \) energy, and \( v_i \) is the velocity of the \( i^{\text{th}} \) energy.

All spectra are then scaled up by the factor \( I_{\text{exp}}/I_{\text{sim}} \).

### 4.1.8 Post Processing and Analysis

Scaled, simulated spectra can be further modified to more realistically correspond with experimental spectra. The two optional modifications in P-FIDAsim are the application of instrumental broadening and the instrumental response function.
Instrumental broadening is the well-known tendency of physical optics to broaden spectral features. Consider, for example, the oxygen V line in Figure 3.2. This line comes from cold oxygen in the edge region and thus, in reality, should look like a spike in this figure. Instead, the sum effect of all optics and electronics is the widening of this line so that it appears greater than 10 Å wide. This effect is taken into account as follows: A Gaussian function is fit to the OV region of the spectrum in Figure 3.2. The DC offset is removed and the amplitude is normalized to 1. The resulting function is the convolution “kernel” such that convolving the kernel and a delta-function-like idealized OV line accurately reproduces the OV region of the experimental spectrum. Applying the instrumental broadening to the simulated spectra then simply amounts to convolving the spectra with this kernel.

The instrumental response function is, in essence, a normalized spectral response to white light. That is, it gives the spectral shape resulting from a source radiating equally at all wavelengths. As such, it takes into account systematic variations in responsivity of CCD elements and, especially here, shows the effect of the neutral density filter designed to filter out most of the cold $D_\alpha$ line. The instrumental response function is then just an array of scaling factors that each spectrum is multiplied by to take this effect into account.

Several analysis codes have been written which consider various outputs of the simulation. For example, one can optimize the ion birth locations considered or the captured ions considered, determine the fast-ion density along each chord, or go on to find the neutral density from experimental spectra.

Optimizing the ion birth locations is about throwing away the vast majority of beam ions; the ones that have a very low probability of entering the chord volumes or making a sizable contribution to the final spectra. This is done by combining the saved outputs from the ion capture module and the atomic loop module. The atomic loop
output contains the emission rate for each captured ion while the ion capture output contains the ion’s original birth location. Combining these results gives photon emission rate as a function of birth location. A cutoff can then be defined in subsequent runs so as to disregard all ions born in certain regions. This is best employed by first running a simulation with a small number of ions (say 50,000), determining the birth location restrictions as described, then running a new simulation with many ions (say 1,000,000) while applying the new restrictions. The result is better statistics and lower simulation run-times. These studies show that the vast majority of emission comes from ions born outside the LCFS, either near the outer wall or near the inner wall.

While optimizing the birth ion locations reduces the number of ion orbits calculated, optimizing the captured ions considered reduces the collisional radiative computational needs. Similar to the above-described method, one can consider photon emission rate as a function of ion location at the time of emission. As such, ions in locations with low emission rates can be excluded from the collisional radiative portion of the code.

Specialized post-processing, like finding the fast-ion density or preparing to find the neutral density, can also be carried out. The fast-ion density along each chord was required for the benchmark tests and is discussed in Section 4.2. Preparation for finding the neutral density involves correlating spectra with the ions’ vertical positions and is discussed in Section 6.1.
Figure 4.4: The effect of the number of beam ions. Applying the instrumental broadening function has significantly smoothed the spectra, hiding the greater noise of the 50k run, however, emphasizing the spectral shape. A sort of convergence is seen near 600k ions. As a compromise, 200k ions were used in the majority of this work while 10 runs of 100k ions each were compiled for the benchmark work discussed in the following section.

4.2 Benchmark Against FIDAsim

P-FIDAsim was benchmarked, or verified, against the well-established FIDAsim code [27] currently used at DIII-D, NSTX, ASDEX, MAST [3][24] and other facilities. The goal of the benchmark is to verify that P-FIDAsim is correctly solving the appropriate mathematical problems. As such, a correlation with experimental scenarios is unnecessary. In fact, the significant differences in purpose and methodologies between FIDAsim and P-FIDAsim require a fairly contrived set of conditions. These conditions, while not realistic, allow the two simulations to consider the same “physical” phenomenon (i.e. overlapping parameter space).
Plasma profiles at DIII-D are expressed in terms of the square-root of the normalized toroidal flux (i.e. $\rho = \sqrt{\Phi_{\text{tor}} / \Phi_{\text{tor,LCFS}}}$, where $\Phi_{\text{tor,LCFS}}$ is the toroidal flux at the last closed flux surface). This normalized flux label is analogous to the minor radius and is a convenient way to cover the (R,z) cross-section with a single variable. Areas having the same value of $\rho$ are called flux surfaces. A parameter, such as electron density, that is equal along a flux surface and varies only when changing $\rho$ is referred to as a flux function.

The parameters of the benchmark (defined as functions of this normalized flux unit) are input to both FIDAsim and P-FIDAsim and are defined as follows. All plasma profiles are uniform inside $\rho = 1.0$ and zero for $\rho > 1.0$. Electron density is $5 \times 10^{12} \text{cm}^{-3}$. Impurity density is zero (i.e. $Z_{\text{eff}} = 1$). Electron temperature and ion temperature are both 100 eV. The equilibrium fields come from DIII-D’s own magnetic equilibrium fitting code called EFIT for shot 152817 at 3000 ms.

The input of the fast-ion population requires more care. The reason is that FIDAsim requires the input of a toroidally-symmetric fast-ion distribution function while P-FIDAsim expects the orbits or capture locations and velocities of individual ions (which is not necessarily toroidally symmetric).

Equivalent inputs were created for both simulations in the following manner: Beam 30-left is used as a starting point for a fast-ion population. To start with, only full-energy 80 keV ions born in the edge region ($R \geq 2.0m$) and near the midplane ($|Z| \leq 3.0cm$) are considered. The orbits are calculated for this small subset of ions. This batch of orbits is then “smeared out” toroidally by replicating the orbits with ever-increasing toroidal angles. The result is a small but toroidally-symmetric fast-ion population. The orbits themselves are entered into P-FIDAsim directly. For FIDAsim, the orbits are binned together on a 3-dimensional mesh to produce the fast-ion distribution function required.
The toroidal replication of orbits nullifies the scaling method in normal P-FIDAsim runs (described in Section 4.1.7). A new scaling method is thus developed just for this special benchmark run and amounts to verifying and forcing both simulations to receive the same inputs. In particular, the fast-ion and edge-neutral densities need to be as similar as possible. While FIDAsim defines the fast-ion density everywhere in the form of a fast-ion distribution function, P-FIDAsim only has fast-ion density defined *implicitly* by the capturing of ions within the lines of sight. Fast-ion density is therefore calculated by going back to the ion capture module and giving each ion a unique identifier. The number of unique ions can then be added up in bins along the length of each chord. This fast-ion density (as a function of distance from each lens) is then compared to the fast-ion density found by interpolating FIDAsim’s fast-ion distribution function (and summing over velocities) along the line of sight. By doing a χ² minimization fit of P-FIDAsim’s fast-ion density to FIDAsim’s density, a scaling factor is found for each chord. Applying these scaling factors simply assures that both simulations are receiving very similar inputs.

To get a source of charge-exchange neutrals and since FIDAsim is meant to simulate fast-ion/beam interactions, the chosen source of neutrals is in the volume of the 210-right beam (ignoring divergence). This beam is chosen as the source of neutrals as the “oblique” sightlines intersect its path. The beam is given virtually no kinetic energy (50 eV) and zero temperature. The neutral density for P-FIDAsim is a uniform $1 \times 10^{10} \text{cm}^{-3}$, while FIDAsim’s neutral density has Monte Carlo noise. Correcting for this minor difference in inputs is done by taking a simple line-average of FIDAsim’s neutral density along each line of sight to make a small correction to P-FIDAsim’s otherwise uniform density.

The results of the benchmark are summarized in Figure 4.5. The total average error of P-FIDAsim, taking FIDAsim as the reference, is 13.6% for six chords. Considering
the highly-different purposes and methodologies of these two simulations, this error seems low enough to verify that the passive simulation is indeed correctly solving the correct set of equations.

4.3 Sensitivity Studies

Sensitivity studies were performed to determine how strongly P-FIDAsim depends upon its inputs. Of particular interest, due to their uncertainty, are the effects of varying neutral densities and plasma edge profiles.

4.3.1 Neutral Density

FIDA radiation is linearly proportional to neutral density. Verifying this neutral density dependence is a simple check that looks for obvious coding errors. Figure 4.6 shows two simulation runs for two chords where the only difference is that the neutral density input was doubled in one case. By dividing the two spectra, the exact factor of two is recovered (Figure 4.6(c)), proving that P-FIDAsim outputs are exactly linear with neutral density.

Next, the sensitivity of the simulation to the spatial distribution of neutral density is considered. Recall from Section 4.1.3 that P-FIDAsim assumes neutral density to be a flux function. Considering the plasma exhaust from the x-points, it is suspected that the neutral density also has a spatial dependence with higher density in the divertor regions. While the simulation records the position of radiating neutrals, the only experimental variation to consider is intensity versus chord viewing location. In looking at the integral of spectra over wavelength, it was noticed that, for shot 152817, the intensity as a function of chord varies oppositely for the experimental
Figure 4.5: Comparison of simulation results for FIDAsim and P-FIDAsim. (a) Sample spectra for oblique chord P9a. (b) Sample spectra for oblique chord P9b. (c) P-FIDAsim results normalized by FIDAsim results for all six outermost chords. The average (RMS) difference is 13.6%.
Figure 4.6: Effect on simulation results of doubling neutral density profile. Simulation of shot 149954 at 3800ms with beam 30-left as the fast-ion source. (a) Effect on chord P6. (b) Effect on chord P8. (c) Ratio of spectra for each chord.

and simulated spectra (compare the upper and lower black curves in Figure 4.7). The average experimental intensity goes down for increasing chord number. While increasing chord number means increasing the average radial location of the chord, another effect is suspected: increasing chord number means the region where the chord intersects the edge region rises further away from the bottom divertor (see circled region of inset in Figure 4.7). This experimental observation helps to solidify the hypothesis that the neutral density increases away from the midplane (for the case of double x-points). P-FIDAsim was then used to test this hypothesis by adding a vertical dependence to the neutral density.
Figure 4.7: Inset: the region of emission suspected of producing the z-dependence. The upper plot is the experimental intensity (averaged over wavelength) versus chord number for shot 152817. Larger chord number equates to larger radial position and higher vertical position (see inset). The lower black curve is the simulated intensity (averaged over wavelength) versus chord number for the same shot with neutral density as a flux function. The lower red curve is the simulated value where the neutral density is given the z-dependence of Figure 4.8 (i.e. increasing downward).
Figure 4.8(a) shows the typical neutral density profile used in the early simulation runs for this work (prior to the neutral density model of Section 4.1.3). This simple flux function does not vary with z but is used as a starting point for a neutral density that does vary with z.

For the study of the spatial dependence of neutral density, a spatially-varying density is created in the following manner. A linear dependence on z is imposed for narrow ranges of $\rho$ such that density at the lower wall ($z \sim -1.35m$) is $\sim 10 \times$ the density at the upper wall ($z \sim 1.35m$), maintaining the same relative $\rho$-dependence. Figure 4.8(b) shows the new dependence on z by grouping the z-values into four groups and plotting density versus $\rho$.

The red spectra in Figure 4.9 are the result of running P-FIDAsim with the spatially-dependent neutral density while the black spectra use the flux-functional form. While spectra simply depend linearly on neutral density, this is true for each small volume along the line-of-sight. This, along with the non-uniform pitch-angle distribution allows not only the amplitude but the shape of the spectra to be altered by the spatial changes in the neutral density. Figure 4.9 shows that adding the z-dependence to the neutral density affects the amplitude as well as the shape of spectra. This sensitivity to neutral density and its spatial distribution is what suggests using first-orbit ions as a known source of fast ions to calculate the edge neutral density profile (discussed in Section 6.1).

The average over wavelength of Figure 4.9 versus chord number is shown as the red curve in the lower plot of Figure 4.7. This curve now more closely matches the trend in the experimental trace above it, strongly suggesting that the hypothesis of increasing neutral density away from the midplane is correct.
4.3.2 Edge Plasma Profiles

The success of P-FIDAsim depends heavily on knowing the plasma profiles in the edge region. However, plasma profiles are not well-known at DIII-D beyond $\rho = 1.0$ and are only measured during specific, concerted campaigns. For most of this thesis work, edge profiles were determined by extrapolating core profiles into the edge region. Thus, sensitivity studies were performed to determine the effects of systematic changes in the edge profiles.

The black curves in Figure 4.10 show typical plasma profiles used for simulations. The red curves show the variation in the extrapolation regions used for this sensitivity study. Table 4.1 summarizes the net effect on spectra from changing the edge profiles. Note that a 361% increase in the edge value of the electron temperature only changes the spectra by $\sim 2 - 6\%$. A 45% decrease in the ion temperature has no real effect on the spectra. By far, the greatest effect on spectra is the change in the electron density edge profile. Increasing edge electron density increases electron-impact ionization of the incoming beam—causing more ion deposition in the edge that later enters the LOS—and also affects the stimulated excitation and relaxation of the fast neutrals. Fortunately, the well-established techniques of Thompson Scattering and Langmuir probes measure electron density to much greater precision than the variation in Table 4.1. Increasing the edge carbon density increases the edge ion deposition by charge exchanging with beam neutrals. Any increase in beam ion deposition in the outer regions leads to greater light pickup by the passive views as ions born in the edge region are on poorly confined orbits that take them near the edge.

As an example of how changing edge profiles changes spectral shape, Figure 4.11 shows how the electron density profile change affects the spectra.
Table 4.1: Effects of the profile changes shown in Figure 4.10. Numbers are in average percentage change with the sign indicating a rise or decline of the parameter.

<table>
<thead>
<tr>
<th>Profile</th>
<th>Profile Change</th>
<th>P1</th>
<th>P3</th>
<th>P5</th>
<th>P7</th>
<th>P9</th>
<th>P11</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_e$</td>
<td>+361</td>
<td>-5.2</td>
<td>-5.2</td>
<td>-6.5</td>
<td>+5.5</td>
<td>+2.8</td>
<td>-2.4</td>
</tr>
<tr>
<td>$T_i$</td>
<td>-45</td>
<td>$\sim 10^{-6}$</td>
<td>$\sim 10^{-6}$</td>
<td>$\sim 10^{-6}$</td>
<td>$\sim 10^{-6}$</td>
<td>$\sim 10^{-6}$</td>
<td></td>
</tr>
<tr>
<td>$n_e$</td>
<td>+245</td>
<td>+125</td>
<td>+116</td>
<td>+178</td>
<td>+46</td>
<td>-10</td>
<td>+18</td>
</tr>
<tr>
<td>$n_e$</td>
<td>+226</td>
<td>+11</td>
<td>+14</td>
<td>+18</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>$n_n$</td>
<td>See Figure 4.8</td>
<td>n/a</td>
<td>+136</td>
<td>+98</td>
<td>+62</td>
<td>-31</td>
<td>-80</td>
</tr>
</tbody>
</table>

Figure 4.8: Edge neutral density dependence. (a) Typical profile is independent of vertical position. This profile is extrapolated from Figure 12 of reference [5]. (b) $z$-dependence added for sensitivity studies. To save computational time, the original function (a) is altered after the ion-capture phase, which means that the density function is only calculated and shown for the location of each captured ion, thus explaining the choppiness seen in (b).
Figure 4.9: Results of adding a z-dependence to neutral density. Notice that both shape and amplitude change. Simulations are of shot 152817 at 3001 ms.
Figure 4.10: Edge profile changes used for sensitivity studies. Profiles for $\rho \leq 1.0$ are fits to data for shot 152817 at 3001 ms. Profiles in the region $\rho > 1.0$ are arbitrary extrapolations of the form $F = F_0 \rho^{-\alpha}$ where $F$ is the profile in question and $F_0$ is that profile’s value at $\rho = 1.0$. $\alpha_{\text{original}}$ is the normal value used for this shot while $\alpha_{\text{new}}$ is used in this edge-profile sensitivity study.
Figure 4.11: Spectra changes from applying the changes to the electron density profile shown in Figure 4.10.
Chapter 5

Comparison with Experiment

This chapter first considers four cases where simulation results correlate well with experimental results and then looks at correlations for all runs as a whole.

5.1 Some Sample Cases

Figure 5.1 shows a few sample comparisons between the simulations and the experiments. The lack of calibration for the spectrometer camera forces these plots to be in arbitrary units. However, it can be seen that several features of the experimental signals are reproduced by P-FIDAsim. For example, all four cases recreate the appropriate overall Doppler shifts. Figure 5.1(a) reproduces the doublet of the main peak as well as the matching amplitude across the neutral-density filter region. Figure 5.1(b) matches the spectral shape very well and contains the experimentally-observed shoulder in the left region of the main peak. A poor experimental signal to noise ratio (SNR) can be seen in Figure 5.1(d), however, the spectral shapes are still similar. Low SNR is a common challenge throughout the dataset, but is particularly
low for the so called “vertical” views due to their lower optical throughput.

Figure 5.1: Comparison between simulation and experiment, showing some of the various correlations. All are in arbitrary intensity units. Experimental spectra are smoothed using a moving average with a width of 2 Å. Note that missing regions in the simulated spectra can be considered zero values as no photons were detected. Spectra were normalized by their maximum values. A systematic red-shift of the simulated spectra can be seen. Much of this is attributed to the necessary use of an out-dated instrumental response function (producing the central drop due to the neutral density filter), which has possibly shifted over time.

5.2 Database of All Cases

This section attempts to quantitatively compare all experiment / simulation pairs. Even if the spectra were calibrated, comparing the entire spectrum is not necessarily the best approach as some areas of a spectrum might correlate well while others do
Therefore, the data presented in this section are created by breaking up each spectrum into narrow regions of wavelength and comparing those regions.

First, some sort of effective calibration factor is required in order to have a self-consistent dataset. That is, a given chord should have the same calibration from shot to shot. These “calibration factors” are found in the following way: All simulated spectra for a given chord are scaled to their corresponding experimental spectra by minimizing the $\chi^2$ between them. The mean of all scaling factors for a given chord is then the scale used for that chord. In this manner, a full set of similarly-valued experimental and simulated spectra are obtained and ready for analysis.

Next, a uniform method of analysis is developed. The method used is to break up each spectrum (both experimental and simulated) into fixed wavelength-bin widths (10 pixels is used, which is about 5 Å). Then each bin (or sub-spectrum) is integrated, giving something like the average spectral value in each narrow region. This means that each pair of experimental and simulated spectra become a set of data points that can be compared to each other. Comparison consists of calculating the Spearman rank correlation coefficient ($R$), where $R = 0$ means a completely random dataset while $R = 1$ indicates a perfect correlation between the two variables. Various parameters are considered to group datasets together to test their correlation as a function of the changing parameter.

Several parameters are varied to produce a dataset of 49 spectral integration time windows. Six of those cases are unusable due to data corruption or other issues, leaving a total of 43 distinct experimental sets. Each of these 43 cases uses two views into the plasma and therefore there are 86 experimental spectra. Each of these 86 cases is simulated using P-FIDAsim. The parameters changed to produce these different cases are: fast-ion source beam, line of sight, plasma current, plasma current slope, and toroidal magnetic field. In post-experimental data analysis, several other
categories can be considered as well. For example, signal integration time, peak signal levels, plasma shape, and even information that only comes from the simulation like ion location at the time of emission.

Note that several parameters are not greatly varied due to experimental restrictions. For example, most datasets are taken at the end of shots designated for a purpose other than passive FIDA light detection. Plasma conditions like density, current, and toroidal field cannot be changed arbitrarily quickly without destabilizing the plasma. In fact, several shots ended in rapid, catastrophic plasma instabilities due to attempting rapid changes in equilibrium parameters.

Figure 5.2 shows four of the more highly-correlated sets of data as examples. Tables 5.1 and 5.2 summarize the data for all cases. Even though some cases are not highly populated (as indicated by single parameter values where there should be a range), several trends are apparent. The higher the experimental signal level, for example, the higher the correlation with the simulation as is seen in the peak signal level and average signal-level correlation coefficients in Table 5.1 (the drop in $R$ for the highest average experimental signal is due to outliers from line leakage). This makes sense as it alludes to the discussion of SNR challenges with this technique. Also related to signal level and SNR is the signal integration time, which also shows a better correlation with higher integration times. There is a greater correlation the more positive the plasma current slope becomes. There seems to be a “preference” for a more triangular plasma (tritop and tribot), which may go along with greater elongation (kappa). Greater elongation or triangulation may be important as it pushes the plasma core closer to the higher neutral-density regions near the x-points.

Some trends in Tables 5.1 and 5.2 are not as easy to see and therefore are benefited by a separate plot. For example, correlation appears to favor lower density as can be seen in Figure 5.3.
In conclusion, many different parameters were changed and modeled. Throughout these variations, the model works well and reproduces the majority of the experimental features.

![Graphs showing correlation](image)

Figure 5.2: Four of the more highly-correlated categories. R is the Spearman rank correlation coefficient. (a) Correlation for a narrow range of a measure of the triangularity of the LCFS in the upper region of the tokamak. Correlation is higher for higher triangularity. (b) Length of time over which signal is integrated (c) Peak of experimental spectra (in a.u.) (d) Chord setup 4 (i.e. chords P6 & P8).
<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
<th>R</th>
</tr>
</thead>
<tbody>
<tr>
<td>All data (full integrals)</td>
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<td>0.58</td>
</tr>
<tr>
<td>All data (partial integrals)</td>
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<td>0.57</td>
</tr>
<tr>
<td>Peak Experimental Signal (a.u.)</td>
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</tr>
<tr>
<td></td>
<td>114.6</td>
<td>0.79</td>
</tr>
<tr>
<td></td>
<td>143.7</td>
<td>0.74</td>
</tr>
<tr>
<td></td>
<td>191.5-226.2</td>
<td>0.80</td>
</tr>
<tr>
<td>Average Experimental Signal (a.u.)</td>
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</tr>
<tr>
<td></td>
<td>6.1-8.8</td>
<td>0.65</td>
</tr>
<tr>
<td></td>
<td>12.6-15.5</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td>20.3</td>
<td>0.80</td>
</tr>
<tr>
<td></td>
<td>23.9-28.5</td>
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</tr>
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</tr>
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<td>30-right</td>
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</tr>
<tr>
<td></td>
<td>150-left</td>
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<tr>
<td></td>
<td>210-right</td>
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</tr>
<tr>
<td></td>
<td>330-left</td>
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</tr>
<tr>
<td></td>
<td>330-right</td>
<td>0.53</td>
</tr>
<tr>
<td>Avg. Plasma Current (MA)</td>
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</tr>
<tr>
<td></td>
<td>0.4-0.5</td>
<td>0.53</td>
</tr>
<tr>
<td></td>
<td>0.7-0.8</td>
<td>0.61</td>
</tr>
<tr>
<td></td>
<td>0.8-1.0</td>
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</tr>
<tr>
<td></td>
<td>1.0-1.2</td>
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</tr>
<tr>
<td>Signal Integration Time (sec)</td>
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<tr>
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<td>0.5-0.8</td>
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<tr>
<td></td>
<td>1.0-1.1</td>
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<tr>
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<td>1.5</td>
<td>0.70</td>
</tr>
<tr>
<td></td>
<td>1.7-2.0</td>
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<tr>
<td>Chord Setup</td>
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<tr>
<td></td>
<td>2 (V1, V2)</td>
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</tr>
<tr>
<td></td>
<td>3 (P8, P10)</td>
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<td></td>
<td>4 (P6, P8)</td>
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<tr>
<td></td>
<td>5 (P2, P4)</td>
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<tr>
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<td>-0.15 - -0.01</td>
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</tr>
<tr>
<td></td>
<td>-0.01-0.14</td>
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<td>0.14-0.28</td>
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<tr>
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<td>0.28-0.43</td>
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<tr>
<td>Right beams</td>
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</tr>
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<td>Plasma Current Slope</td>
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<td>constant</td>
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<tr>
<td></td>
<td>ramping down</td>
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Table 5.1: Summary of database analysis, Part 1. Values are time-averaged. R is the Spearman rank correlation coefficient from scatter plots like those in Figure 5.2.
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<thead>
<tr>
<th>Description</th>
<th>Value</th>
<th>R</th>
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<td>Density ((densv3) \times 10^{19} m^{-3}) (see Figure 5.5)</td>
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<td></td>
<td>1.3-1.6</td>
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<tr>
<td></td>
<td>1.6-1.9</td>
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<td></td>
<td>2.0-2.3</td>
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<tr>
<td></td>
<td>1.6-1.7</td>
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</tr>
<tr>
<td></td>
<td>1.9-2.0</td>
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</tr>
<tr>
<td></td>
<td>2.1-2.3</td>
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<tr>
<td></td>
<td>2.5-2.7</td>
<td>0.41</td>
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<tr>
<td>Density ((densv2) \times 10^{19} m^{-3}) (see Figure 5.5)</td>
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<tr>
<td></td>
<td>1.4-1.6</td>
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</tr>
<tr>
<td></td>
<td>1.6-1.9</td>
<td>0.57</td>
</tr>
<tr>
<td></td>
<td>1.9-2.2</td>
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</tr>
<tr>
<td></td>
<td>2.2-2.5</td>
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</tr>
<tr>
<td>Average Toroidal Field (T)</td>
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</tr>
<tr>
<td></td>
<td>-0.514 - -0.511</td>
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</tr>
<tr>
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<tr>
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<td>0.083-0.092</td>
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<td></td>
<td>0.092-0.102</td>
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<tr>
<td></td>
<td>0.102-0.111</td>
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<td>Shape Factor (kappa) (see Figure 5.4)</td>
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<td>1.601-1.632</td>
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<tr>
<td>Shape Factor (tritop) (see Figure 5.4)</td>
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<tr>
<td></td>
<td>0.032-0.051</td>
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<tr>
<td></td>
<td>0.063-0.082</td>
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</tr>
<tr>
<td></td>
<td>0.098-0.105</td>
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</tr>
<tr>
<td></td>
<td>0.138</td>
<td>0.57</td>
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<td>Shape Factor (tribot) (see Figure 5.4)</td>
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<tr>
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<td>0.028-0.044</td>
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<td></td>
<td>0.057-0.076</td>
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<tr>
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</tr>
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<td></td>
<td>P10</td>
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</tr>
<tr>
<td></td>
<td>V1</td>
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</tr>
<tr>
<td></td>
<td>V2</td>
<td>0.60</td>
</tr>
</tbody>
</table>

Table 5.2: Summary of database analysis, Part 2. Values are time-averaged. R is the Spearman rank correlation coefficient from scatter plots like those in Figure 5.2.
Figure 5.3: Spearman rank correlation coefficient between experiment and simulation vs. electron density (with a quadratic fit).
Figure 5.4: Equilibria illustrating extreme shape factor values from Table 5.2. Elevation views show chamber wall, contours of $\rho$, and LCFS (blue). The shape factors describe the LCFS. Upper Left: gapout is the distance between the LCFS and the outboard wall in meters. Upper Right: kappa is the elongation (height/width). Lower Left: tribot is a measure of the triangularity of the LCFS in the lower region. Lower Right: tritop is a measure of the triangularity of the LCFS in the upper region.
Figure 5.5: Location of interferometer chords giving densities in Table 5.2 (with sample equilibrium and LCFS).
Chapter 6

Applications of Passive FIDA

Thus far, the use of passive FIDA measurements to identify (and, with the help of P-FIDAsim, quantify) first-orbit light has been addressed. This chapter goes beyond that application to discuss how the inversion of simulated spectra and the use of experimental data infers the neutral density; how the inversion method is tested and optimized; and will present the resulting neutral density profile. Some thoughts are also presented on how passive FIDA light and P-FIDAsim together can be used as a generalized fast-ion loss diagnostic.

6.1 Neutral Density Measurement

As shown in Section 4.3.1, passive FIDA spectra depend linearly on the background (mostly edge) neutral density. If the neutral density is known for a given experiment or, better yet, measured every shot, then P-FIDAsim will return quantitative absolute spectra. These spectra can then be used to quantify beam losses from the charge exchange of first-orbit ions or fast-ion losses in general (Section 6.2). Many fusion
research devices, however, do not have regular measurements of the neutral density. In this case, P-FIDAsim can use beam first-orbit light to estimate the neutral density.

Attempts were made to measure the neutral density during the shots allotted for this work using a more traditional method of the tomographic inversion of $D_\alpha$ and $D_\gamma$ emission. Absolute simulated spectra could then be compared to calibrated experimental spectra for the validation of P-FIDAsim. However, various experimental difficulties conspired to prevent the measurement of the neutral density. Having successfully obtained one calibrated set of good spectra, the validation of P-FIDAsim was chosen to be the determination of the neutral density using first-orbit light. This process, therefore, serves to validate the entire passive FIDA simulation and also works as a proof of principle for this method of neutral density measurement.

The specific data used to find the neutral density are as follows. Shot number 152817 uses beam 30-left as a modulated fast-ion source. Beams 150-right and 330-right are active for small amounts of time to maintain the equilibrium and, therefore, these times are ignored. Calibrated spectra are collected by the HoloSpec spectrometer for views P1, P3, P5, P7, P9, and P11 (see Figure 6.3). Spectra are time-averaged from 1800 ms to 4600 ms. The profiles and equilibrium are taken to be those at 3001 ms.

P-FIDAsim self-consistently calculates the normalized neutral density flux function over R and z (as per Section 4.1.3). Recall that the scaling (the source) of this neutral density is a free parameter and that neutral density is not simply a flux function. Because neutrals do not respond to magnetic fields, neutral sources and sinks freely cause spatial variations that alter the neutral density and prevent it from having a flux-functional form. DIII-D, having a well-conditioned first wall, is assumed to have a uniform neutral source rate everywhere except in the actively-pumped divertor regions. Shot 152817 has double x-points and therefore has higher neutral ejection from the core and pumping in the upper and lower regions. For this
reason, a z-dependence is assumed for the neutral density, the nature of which will be determined by the following inversion process.

### 6.1.1 Inversion Overview

The purpose of the inversion process is to solve the over-determined least-squares optimization that essentially finds the neutral-density scaling (or source) factor (as a function of z) that minimizes the difference between the simulated and experimental spectra. The 2D grid of normalized neutral density is then multiplied by this scaling factor to obtain a neutral density that is scaled to realistic values and has a functional form in $\rho$ and z (in practice, R and z).

This application of P-FIDAsim requires the z-position of each neutral at the time of emission and therefore does not use the usual output from the spectra module. Instead, the output of the ion capture module (which contains the requisite fast-neutral locations and velocities) is combined with the output of the atomic loop module, which provides the photon emission rate and shifted wavelengths. Instead of binning together all photons in a given LOS to make a single spectrum for a single chord (producing the usual nChords number of spectra), this portion of the code bins first in vertical position, z. The new output is a spectrum for each z-bin for each chord (i.e. nChords \times nZbins spectra). This retention of the vertical position data is what makes the inversion possible.

The inversion has three terms: The unknown neutral density scaling factor $\alpha$ as a function of z, the experimental spectra $E$ as a function of wavelength and chord number, and the simulated spectra $S$ as a function of wavelength, chord number, and z. Let there be $nw$ wavelength bins in each spectrum, $nc$ chords, and $nz$ vertical bins. Ignoring the LOS, or chord, designation, all chord data is lumped together as
one large dataset. Noting that subscripts refer to a given wavelength, chord, or z-bin, not the matrix-element location, the three terms are defined as:

\[
\alpha(z) = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_{nz} \end{bmatrix},
\]

\[
E(\lambda) = \begin{bmatrix} E_{1,1} \\ E_{2,1} \\ E_{3,1} \\ \vdots \\ E_{nw,1} \\ E_{1,2} \\ E_{2,2} \\ E_{3,2} \\ \vdots \\ E_{nw,2} \\ \vdots \\ E_{nw,nc} \end{bmatrix},
\]

\[
S(\lambda, z) = \begin{bmatrix} S_{1,1,1} & S_{1,1,2} & S_{1,1,3} & \cdots & S_{1,1,zn} \\ S_{2,1,1} & S_{2,1,2} & S_{2,1,3} & \cdots & S_{2,1,zn} \\ S_{3,1,1} & S_{3,1,2} & S_{3,1,3} & \cdots & S_{3,1,zn} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ S_{nw,1,1} & S_{nw,1,2} & S_{nw,1,3} & \cdots & S_{nw,1,zn} \\ S_{1,2,1} & S_{1,2,2} & S_{1,2,3} & \cdots & S_{1,2,zn} \\ S_{2,2,1} & S_{2,2,2} & S_{2,2,3} & \cdots & S_{2,2,zn} \\ S_{3,2,1} & S_{3,2,2} & S_{3,2,3} & \cdots & S_{3,2,zn} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ S_{nw,2,1} & S_{nw,2,2} & S_{nw,2,3} & \cdots & S_{nw,2,zn} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ S_{nw,nc,1} & S_{nw,nc,2} & S_{nw,nc,3} & \cdots & S_{nw,nc,zn} \end{bmatrix}.
\]

Because the experimental signals are line-integrated, the key equation to invert then becomes

\[
E = S\alpha.
\] (6.1)

Inverting this equation amounts to a least-squares fitting, giving the optimal neutral density scaling factors, \(\alpha\):

\[
\alpha = S^{-1}E.
\] (6.2)

The inversion is performed using a generalization of a non-negative least-squares solver [37]. The code allows for arbitrary restrictions to be placed on \(\alpha\). However, non-negative was the only restriction used in this work.
Defining the normalized neutral density, $\bar{n}_n(R, z)$, as

$$
\bar{n}_n(R, z) = \begin{bmatrix}
\bar{n}_{1,1} & \bar{n}_{1,2} & \bar{n}_{1,3} & \ldots & \bar{n}_{1,n_R} \\
\bar{n}_{2,1} & \bar{n}_{2,2} & \bar{n}_{2,3} & \ldots & \bar{n}_{2,n_R} \\
\bar{n}_{3,1} & \bar{n}_{3,2} & \bar{n}_{3,3} & \ldots & \bar{n}_{3,n_R} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\bar{n}_{nz,1} & \bar{n}_{nz,2} & \bar{n}_{nz,3} & \ldots & \bar{n}_{nz,n_R}
\end{bmatrix}
$$

and replicating the columns of $\alpha$ $n_R$ times (and calling it $\alpha'$) to produce the $n_z \times n_R$ matrix

$$
\alpha'(z) = \begin{bmatrix}
\alpha_1 & \alpha_1 & \alpha_1 & \ldots & \alpha_1 \\
\alpha_2 & \alpha_2 & \alpha_2 & \ldots & \alpha_2 \\
\alpha_3 & \alpha_3 & \alpha_3 & \ldots & \alpha_3 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\alpha_{nz} & \alpha_{nz} & \alpha_{nz} & \ldots & \alpha_{nz}
\end{bmatrix},
$$

gives the best estimate of the neutral density (multiplying element by element) of:

$$
n_n(R, z) = \bar{n}_n \circ \alpha'.
$$

### 6.1.2 Inversion Optimization

Testing and optimizing the inversion process consists of determining if the method reproduces the neutral density within acceptable error limits and how many vertical $z$-bins should be used to minimize that error.

The inversion tests are designed not only to verify the general method but also to optimize the specific neutral density calculation discussed in Sections 6.1 and 6.1.3.
Therefore, the inversion tests are carried out using the same conditions, equilibria, and profiles from shot number 152817 that will be used for that particular experimental determination of the neutral density.

To conduct the test, three items are needed: 1. a known neutral density 2. a set of calibrated experimental spectra and 3. a corresponding set of simulated spectra (that employ a normalized neutral density). The way to test the inversion process which introduces the least amount of uncertainty is to construct these three elements computationally.

First, the “known” neutral density is created. This is done by starting with the normalized neutral density as a function of R and z found by P-FIDAsim (Section 4.1.3). An arbitrary but known vertical functional form is then used to alter and scale the normalized neutral density. A physical and a computational justification are invoked in assuming the neutral density rises symmetrically away from the midplane (i.e. that \( \alpha(z) = \alpha(|z|) \)). Physically, as already discussed, the double x-point of this equilibrium suggests increasing neutral density away from the midplane. Computationally, the inversion is unstable if positive and negative z values can have independent densities. This makes sense when considering that the lines of sight pass through the upper and lower regions a similar amount and simply integrate the signals. The inversion, therefore, cannot “tell the difference” between light emitted in the upper regions and light emitted in the lower regions. This computational instability is expected to go away for single x-point cases. Symmetry about \( z = 0 \) is thus imposed and (for this inversion test) the arbitrary scaling factor used is: \( \alpha = 7 \times 10^{13} \times |z| + 1 \times 10^{13} \), thus putting the neutral density into units of \( cm^{-3} \). The normalized neutral density times this input \( \alpha \) gives an exactly-known neutral density. Note the difference between this perfectly-known input \( \alpha \) and the \( \alpha \) found by inversion. This input \( \alpha \) is used only for this contrived test and is not normally known or used.
A simulation is run for all six chords using this “known” neutral density. This run is then considered to be the “experimental” run (E in Equation 6.1).

The simulation using the normalized neutral density (in the usual manner) is considered the “simulation” run (S in Equation 6.1) while $\alpha$ remains the unknown to be determined by inversion.

The only remaining variable is the number of z-bins (nZbins) in which to collect the CX neutrals. While the number of z-bins is arbitrary, there is an interplay between nZbins and the inherent spatial resolution and, especially, the chord-spacing and the height-change from chord to chord of the region of greatest emission. For example, two z-bins would not give enough useful information while one hundred z-bins would be impossible for six chords to resolve.

Thus, the inversion test was carried out for several values of nZbins. Figure 6.1 shows the results of running the test as a function of nZbins. The error reported is the simple RMS error of the input $\alpha$ function compared to the output $\alpha$ function. However, this is the exact same error as the RMS error of the entire (R,z) neutral density contour and, therefore, is the overall error of the inversion process. As indicated by the “×” in Figure 6.1, $nZbins = 5$ was chosen for the final determination of the experimental neutral density (discussed in Section 6.1.3).

Figure 6.2 shows the results of the inversion test for the $nZbins = 5$ case. While five vertical bins were used, only four contained emitting neutrals and therefore made it to Figure 6.2. The red line is a simple, linear interpolation and extrapolation of these four data points. It is this interpolation/extrapolation that is compared to the input $\alpha$ function to get the error of 4.8% shown in Figure 6.1.

The inversion method is thus shown to introduce less than 5% error in calculating the neutral density and five vertical bins is shown to be a judicious choice in this
particular case.

![Graph showing RMS error of alpha scaling factor as a function of number of vertical bins.](image)

Figure 6.1: Error in inversion process as a function of number of vertical bins. “×” marks value used to find neutral density ($n_{Zbins} = 5$).

### 6.1.3 Inversion Results

Figure 6.3 shows the experimental spectra used to find the DIII-D neutral density. Figure 6.5 shows the same experimental spectra with the wavelength bases trimmed as they are for the inversion. The figure also includes the simulated spectra after being scaled by the neutral density. Figure 6.4 shows the $\alpha$ found by inversion. Note that it rises quickly away from the midplane, as hypothesized. To again emphasize the role of the neutral density’s spatial distribution in shaping the fast-ion spectra, Figure 6.6 shows the simulated spectra before and after the neutral density scaling.

Figures 6.7-6.10 serve as the experimental validation of the passive FIDA simulation as a whole. Figure 6.7 is a contour plot of the neutral density obtained. Two basic features are obvious in comparing this contour to that of the normalized contour of
Figure 6.2: Scaling factor $\alpha$ found by inversion test compared to the input $\alpha$.

Figure 4.3: the scaled neutral density has realistic values and the z-dependence is made apparent by the low densities closer to the midplane. Figure 6.8 compares the poloidally-averaged neutral density (as a function of $\rho$) found by P-FIDAsim and a measured neutral density found some 15 years earlier by Carreras et al. [5]. Considering the temporal and situational differences, exact correlation is not expected, however, the order-of-magnitude correlation is excellent. Figure 6.9 compares the same two works again, this time expressing neutral density along the LCFS as a function of poloidal angle. Again, the order-of-magnitude correlation is excellent and the figure goes further by showing that the calculated neutral density also peaks at the x-points. Figure 6.10 shows the results of a DEGAS calculation that was used to calculate the neutral flux into the core along the LCFS [6]. For comparison, the P-FIDAsim output was converted to a neutral flux by multiplying by the velocity normal to the LCFS. The results are similar in amplitude and both show the characteristic peak at the x-point(s).
Figure 6.3: Calibrated, experimental spectra of passive FIDA from first-orbit ions used to find the neutral density. Note the negative values at 6500 Å due to imperfect oxygen V line removal in the time-slice subtraction. These negative values are not used in the inversion as they result in negative neutral densities.

### 6.2 Detecting Fast-Ion Losses from Instabilities

Passive FIDA measurements can be used to quantify losses other than first-orbit losses. This section will briefly introduce the general use of such measurements and will also address the possible role of P-FIDAsim in such applications.

In principle, edge fast-ion losses resulting from any instability that are accompanied by a fluctuation in a measured quantity can be quantified using passive FIDA techniques. The time-varying parameter is required in order to conditionally average the spectra. As an example, consider the sawtooth instability. While, in the study of first-orbit light, the modulated beam power is the periodic signal used for conditional averaging, in the case of sawteeth, it is the plasma temperature that is fluctuating. The sawtooth is a good example as it is a common loss mechanism in tokamaks and occurs in many
Figure 6.4: Alpha neutral density scaling factor found for shot 152817.

of the shots collected for this work.

The sawtooth instability is a periodic relaxation of the electron and ion temperature profiles [16]. As seen in Figure 3.6(a), the electron temperature (as seen by the ECE signal) rises relatively slowly and crashes quickly. The sudden drop in temperature is due to hot particle ejection from the core into the edge region via magnetic reconnection. As such, at the times that the core temperature is dropping, the edge temperature is increasing. Therefore, the sawtooth can be said to have a location (the inversion location, referred to as $\rho_{\text{inversion}}$) where the temperature does not change. Inside $\rho_{\text{inversion}}$ the temperature drops with every crash and outside $\rho_{\text{inversion}}$ the temperature rises with every crash. A crash also has an amplitude, which can be defined as the fraction of core temperature drop (i.e. $(T_{e,\text{core before crash}} - T_{e,\text{core after crash}})/T_{e,\text{core before crash}}$).

Sawtooth loss spectra are created by conditionally averaging raw spectra. This is done by averaging all spectra immediately after each sawtooth crash and subtracting from
that the average of all spectra immediately before each crash. An example can be seen in Figure 6.11. Interpretation is more difficult here than with first-orbit light as both impurity lines and the Bremsstrahlung background rise due to the edge heating. This means that analysis should only be done after removing a best estimate of the Bremsstrahlung level and should avoid known impurity line regions. The regions of the spectrum possibly resulting from fast-ion losses are marked in Figure 6.11. Because the viewing geometry is largely tangential, the greater level of blue signal over red is consistent with the mostly co-going fast-ion population of this shot.

To further test the plausibility that the experimental data in Figure 6.11 does in fact contain FIDA signals from sawtooth-crash-ejected fast ions, the TRANSP code [38] is run for the same shot and conditions to determine the fast-ion distribution function, \( F \). Fast ions inside the sawtooth inversion radius are summed to obtain an estimate of ions that could be expelled to the plasma edge, \( F(E,p) \), where \( E \) is the fast-ion energy and \( p = \frac{v_\parallel}{v} \) is the pitch. Next, FIDASim is used to calculate weight functions [39][40], \( W(E,p;\lambda) \), for the views in question. Usually, FIDASIM employs injected neutrals but, in this special calculation, the injected neutrals were replaced with cold neutrals as in the benchmark with P-FIDASim (Section 4.2). The spectra for the desired chords are the integral of the product of \( F \) and \( W \), i.e. \( S = \int FWdEdp \), where the integral is over pitch and energy. One oblique chord, P4, is used and the spectrum is shown in Figure 6.11 and one vertical chord, V1, is used, the integral of which is shown in Figure 6.13. Using the fast-ion distribution function inside the sawtooth inversion radius is a first-order estimate of sawtooth spectra which essentially assumes that sawtooth crashes simply eject a uniform sampling of the fast-ion population into the edge region. This is an over-simplification in several respects. Sawtooth crashes do not simply eject a representative sample of the confined distribution and, in fact, are known to preferentially affect passing particles. Particles redistributed outwardly undergo changes in energy and pitch in the process and therefore do not represent
the confined ion distribution. In addition, the TRANSP spectrum shown in Figure 6.11 uses an improvised neutral density spatial profile. However, despite these issues, the TRANSP spectrum has a striking similarity to the experimental spectrum. In particular, the bias towards blue-shifted light is apparent and can also be seen in Figure 6.13.

Losses from sawtooth instabilities can be quantified by comparing them to more-quantifiable losses in the form of first-orbit losses. For a given shot with both first-orbit light and sawtooth-induced light, the plasma and neutral profiles are equivalent, allowing for the direct comparison of these two sources of light. In the case of fast-ion losses, the atomic physics and neutral density are everywhere equal for the two mechanisms and therefore comparing the edge light intensity gives $L_{\text{sawtooth}}/L_{\text{first-orbit}} \approx n_{\text{fast-ion, ST}}/n_{\text{fast-ion, FO}}$.

Figure 6.14 shows an application of sawtooth fast-ion loss detection by quantifying the losses as a function of sawtooth amplitude and location. A direct proportionality is seen in both cases. This means that the greater the reduction in the core temperature, the greater the amount of fast-ion losses to the edge. It is well known that sawteeth redistribute thermal and fast ions outwardly [7][41]. The more internal a sawtooth is (i.e. the smaller $\rho_{\text{inversion}}$ is), the more the ejected particles tend to remain confined, simply altering their distribution. However, as the sawtooth location occurs further out, there is increased probability for particles to be lost. This increase in losses can be seen clearly in Figure 6.14.

Sawtooth crashes are predicted by Kolesnichenko [42] to more heavily affect passing particles than trapped particles. Sawtooth crashes involve magnetic reconnection and alteration of flux surfaces. Passing particles follow field lines closely and so are affected more by the reconnection than trapped particles which shift back and forth over multiple flux surfaces, effectively averaging over the local perturbations.
The increased sensitivity of passing ions to the sawtooth instability has now been measured by FIDA [7][41] and by collective Thomson scattering [43]. Muscatello et al. [7] used the same optics system used for this doctoral work to show the increased effect on passing ions as well as the fact that the vertical views used in this work are more sensitive to trapped ions and the oblique views are more sensitive to passing ions. The reason is simply the relative Doppler shifts. Passing particles have a larger $v_\parallel$, giving them the Doppler shift needed to be seen by the oblique system. Trapped particles have a larger $v_\perp$ and therefore have a more favorable Doppler shift for the vertical system. Figure 6.14 shows a larger average value for the oblique views (i.e. passing ions), consistent with the above-referenced measurements that show the preferential redistribution of passing ions during sawtooth crashes.

The method described thus far is completely experimentally based and can be performed in a large number of scenarios. Simply by modulating a neutral beam that produces first-orbit light in the volume being observed, instability losses can be expressed in terms of first-orbit densities. To go further, if first-orbit densities are quantified in absolute units (by one of several methods) then instability losses can be put into those same units. It may be meaningful to use P-FIDAsim to make such an absolute measure of first-orbit losses.

With a known neutral density profile, P-FIDAsim can output the density of first-orbit fast-ions along each LOS. In practice, it may be most useful to consider a line-integrated value such as the line-averaged fast-ion density per chord. Figure 6.14 can then be put into the same units by using $n_{fast-ion, ST} \approx L_{sawtooth} \times n_{fast-ion, PL} / L_{first-orbit}$.

In fact, the phenomenon is more complicated then this considering the spatial dependence of the pertinent interactions. However, with much (if not most) of the light coming from the edge region (see Figure 6.15), the volumes of emission are actually far more localized than simple chord geometry would suggest and therefore this sim-
ple approach may be a good first-order method of determining fast-ion losses from instabilities.

As a proof-of-principle of this method of loss detection, the fast-ion losses due to the sawtooth instability are estimated for shot 149941 (average per sawtooth from 3485 to 4982 ms using chord P4). Three main components go into this calculation: the amount of sawtooth edge light, the amount of first-orbit edge light, and the line-averaged first-orbit density inside the chord. The sawtooth light is taken as the integral of the “Suspected FIDA Signal” in Figure 6.11 (after removing the Bremsstrahlung offset) and the first-orbit light is taken as the integral of the entire first-orbit spectrum for this scenario (not shown). The ratio of light \( L_{ST}/L_{FO} \) is found to be 6.07. The fast-ion density along the chord, \( n_{fi} \), is found by binning the ions from the ion capture module of P-FIDAsim. However, the first-orbit density, \( n_{FO} \), is not equal to the fast-ion density. Only the fast-ions that charge exchange will be lost and therefore contribute to \( n_{FO} \). While P-FIDAsim could, in principle, track and output CX rates, it does not currently do so. Therefore, the neutral density along the chord is used as a proxy for the CX rate. The first-orbit density is defined as \( n_{FO} = \int n_{fi} n_{n} d\ell / \int n_{n} d\ell \), where the integration is along the length of the chord. The line-averaged first-orbit density is thus estimated to be \( 7.45 \times 10^{15} m^{-3} \) while the sawtooth-induced density \( (n_{FO}L_{ST}/L_{FO}) \) is \( 4.52 \times 10^{16} m^{-3} \). To estimate the total number of ions lost per sawtooth \( (N_{ST}) \), the following assumptions are made: 1. toroidal symmetry (justified by the \( n = 0 \) mode structure of the sawtooth crash), 2. the line-averaged sawtooth loss density represents the global loss density and 3. the loss volume is \( V_{loss} = (2\pi R)(\frac{2}{3} \kappa a) \Delta r_{n} \), assuming a 45° poloidal angle of losses, where \( R \) is the major radius (2.185m), \( \kappa \) is the average elongation (1.160), \( a \) is the minor radius of the LCFS (0.636m), and \( \Delta r_{n} \) is a characteristic neutral density penetration depth (0.211m). This gives a loss volume of \( 1.7 m^{3} \) and the number of lost ions \( (N_{ST} = n_{ST} V_{loss}) \) as \( 7.6 \times 10^{16} \). The TRANSP run gave a fast-ion inventory of
6.3 × 10^{18}, meaning that the sawtooth crashes ejected on average 1.2% of the fast-ions. The TRANSP code includes an optional Kadomtsev [44] model of the sawtooth crash. To assess the reasonableness of the experimental evaluation of the total losses, a representative sawtooth crash in discharge 149941 is simulated using this model. The number of confined fast ions drops 1.7% at the sawtooth crash in the simulation, in good agreement with the experimental estimate.
Figure 6.5: Experimental spectra and simulated spectra after applying the neutral density from inversion. Note: the wavelength bases are all different and are determined by 1. where the experimental spectrum goes negative (at low wavelengths) 2. where the experimental spectrum reaches the end of the CCD array (high wavelengths) and 3. where experimental spectra rise unrealistically due to very high calibration factors resulting from the neutral-density filter (higher wavelengths).
Figure 6.6: Simulated spectra before and after neutral density scaling. The normalized cases are scaled to the maximum of the scaled cases. Note that, because $\alpha$ is a function of $z$, the spectra change shape after scaling.
Figure 6.7: Experimental neutral density from simulation inversion for shot 152817.
Figure 6.8: **Upper Plot**: Poloidally-averaged neutral density at DIII-D as measured by Carreras (Figure 12 of [5]) for various experimental conditions. **Lower Plot**: Poloidally-averaged neutral density for shot 152817 as measured by first-orbit light and P-FIDAsim inversion.
Figure 6.9: **Upper Plot:** Poloidal distribution of neutral density along a flux surface just inside the LCFS at DIII-D as measured by Carreras (Figure 14 of Reference [5]). These experiments had one x-point at 258°. The dark trace is the “standard” case while the dashed lines are raised by a gas puffing. **Lower Plot:** Poloidal distribution of neutral density along the LCFS for shot 152817 as measured by first-orbit light and P-FIDAsim inversion. The two x-points are marked by vertical lines.
Figure 6.10: Upper Plot: Neutral deuterium flux into the core as calculated for DIII-D by Groth using the DEGAS code (Figure 3 of Reference [6]). Lower Plot: The neutral deuterium flux into the core at the LCFS as calculated by P-FIDAsim. The neutral flux is equal to the neutral density at the LCFS multiplied by the average neutral velocity normal to the flux surface. This average velocity is found all along the LCFS using the 1D neutral density model of Section 4.1.3.
Figure 6.11: Spectrum found by conditionally-averaging edge light based on the timing of a core ECE channel during a sawtooth instability (26 crashes found) from shot 149941 (3485-4982 ms, chord P4). Many of the impurity emission lines identified in Figure 3.2 are still present in this spectrum (unlike in first-orbit spectra where the lines subtract out). The presence of impurity lines is explained by the well-known phenomenon of edge-heating due to the ejection of high temperature particles. The edge heating raises and widens the impurity line signals, thus producing an asymmetry in the time-slice subtraction. The conditional averaging uses 3 ms before each crash and 3 ms after each crash. The curve labeled TRANSP is a spectrum produced using the TRANSP distribution function for this shot and time (shown in Figure 6.12). It uses an improvised neutral density profile and essentially assumes that the sawtooth crashes eject the confined ions coherently. The curve is normalized to the experimental curve and is included to show the plausibility of the sawtooth spectrum, especially the bias toward blue-shifted light resulting from the largely co-going ion population.
Figure 6.12: Fast ion distribution output from TRANSP for shot 149941, just inside the sawtooth inversion radius of $\rho = 0.43$. 
Figure 6.13: A comparison of the blue portion of the spectrum and the red for the entire data set of sawtooth loss spectra. Each value is the mean spectral value in ranges equidistant from the cold line (6590 – 6610Å and 6512 – 6532Å). The strong bias towards blue-shifted light for the oblique views is consistent with the use of co-going beams and the greater sensitivity to passing particles. The crude sawtooth spectral model using TRANSP and FIDAsim (shown in Figure 6.11) also shows a blue bias for the oblique chord. The vertical views being more balanced between red and blue is consistent with their greater sensitivity to trapped particles. This spectral balance is further validated by the TRANSP/FIDAsim data point for a vertical chord (which comes from a spectrum analogous to the TRANSP curve in Figure 6.11). The average oblique value (blue + red) is 19.0 while the average vertical value is 3.4, which shows that not only do sawtooth crashes preferentially rearrange the distribution of passing ions, but they also cause greater losses of passing ions. Oblique and vertical signal levels are assumed to be on the same scale as they use the same diameter optic fiber and the same spectrometer, however they have different port windows, lenses, and mirrors, perhaps adding a ≤ 20% error in scaling.
Figure 6.14: Sawtooth losses (compared to first-orbit losses) as functions of sawtooth amplitude and location. Each data point is created by averaging the blue or red region of the sawtooth spectrum and dividing by the corresponding first-orbit average. Blue averages are over the 6510-6550Å region and the red averages are over the 6590-6610Å region. In all cases, there is a direct proportionality. That is, greater reductions in the core temperature result in greater losses to the edge and crashes taking place closer to the edge produce more losses. The $\rho$ dependence is consistent with previous studies showing that more internal crashes allow for more particle redistribution instead of loss. The plots are consistent with studies showing that oblique views are more sensitive to passing ions and vertical views are more sensitive to trapped ions as well as the fact that sawtooth crashes have a larger impact on passing ions [7]. The average blue oblique value is 2.4 while the average blue vertical value is 1.2 (i.e. higher passing ion losses). The average red oblique values is 0.7 while the average red vertical value is 0.9 (i.e. trapped ions cause the majority of the red shift and vertical views are more sensitive to trapped ions).
Figure 6.15: The photon emission rate averaged over all space for all simulation runs, showing that 42% of all light comes from the edge region ($\rho > 1.0$). Many individual cases have much higher fractions of edge light.
Chapter 7

Conclusion and Future Work

This chapter will make some closing remarks and discuss some possible directions for future work in the area of passive FIDA.

7.1 Conclusion

Spectra from fast neutrals born of the charge exchange of first-orbit fast-ions in the edge region has been measured and modeled. The passive FIDA simulation is verified against the established FIDAsim code. The 50 – 80% correlation in spectral shape between experimental and simulated spectra suggest that the observed spectra are indeed from beam first-orbit losses and validates P-FIDAsim to within a single scaling factor (the neutral density). P-FIDAsim was also used to determine the neutral density profile using first-orbit spectra and, while not only showing the greater potential of the simulation, the excellent correlation of the inferred neutral density with experimental measurements and DEGAS simulations also acts as indirect validation of P-FIDAsim. Having established a solid foundation for first-orbit, passive
light measurement and simulation, an introduction was made into the measurement of general fast-ion losses. A method is shown for expressing instability losses relative to first-orbit losses and it is shown that P-FIDAsim can be used to further estimate those losses in absolute units.

### 7.2 Future Work

#### 7.2.1 First-Orbit Modeling

Currently, the main challenge in applying P-FIDAsim is the computational run-time. As mentioned, most of the computation time is spent calculating ion orbits. A proposed improvement, which was explored some during this work, is to use conserved quantities to track a guiding-center orbit in place of the current full orbit. This must be accompanied by the gyro-radius in the ion capture module in order to capture sufficient and realistic numbers of ion orbits in the lines of sight. A straightforward replacement of the full orbit with the guiding-center orbit will capture far too few ions. Once the ions are captured, a gyro-phase and perpendicular velocity can be applied to each ion so as to, in effect, recover the full orbit. This should reduce this portion of the calculation time by 10 to 100 times.

The simulation can be further sped up by converting to Fortran as has been done recently for FIDAsim. The full orbit code currently employed, however, is already in Fortran and uses an IDL wrapper for integration into the rest of the simulation. The real benefit of conversion would therefore be expressed mostly in the collisional-radiative model.

This doctoral work did not require highly-optimized simulation runs. That is, lower
statistical noise was a larger concern than computational run-time. In future applications, a more systematic use of the optimizations discussed in Section 4.1.8, could dramatically reduce computation times. Specifically, most of the birth ions can be ignored and much of the line-of-sight volume can also be ignored.

After carrying out the above optimization, if the volume of the beam to be considered is larger than the volume of the chord to be considered (as is usually the case), then it is more efficient to originate ions inside the LOS and run time backwards to find what ions originate from the beam. The larger the difference in these two volumes, the more this improvement will speed up the calculation.

The DIII-D “oblique” views are each made up of three separate fiber optics with slightly different views. This fact was not taken into account in the main P-FIDAsim runs and was only used in the benchmark codes. Future applications should, of course, contain as realistic geometry as can be obtained.

Several smaller changes could also be made. Presently, the normalized neutral density module is run manually. Future versions should incorporate these codes in the main simulation. The ion capture and atomic loop outputs are large and are not necessary to save if the pertinent values are calculated first. For example, fast-ion density along each chord, spectra as a function of z (for neutral density calculation), and radiance as a function of initial and final positions could all be calculated (perhaps selectively) and the intermediate results discarded. This would minimize the data storage needs of the simulation.
7.2.2 Measurements and Simulation Inputs

As is usually the case in spectroscopic measurements, higher throughput should improve the quality of the fast-ion spectra. Uncertainties are dominated by photon statistics, which rise more slowly than the signal level itself. While considerable effort has been made to create a high-throughput system at DIII-D, it remains a general remark that higher raw signals will only improve these types of measurements.

Passive FIDA light (whether from first-orbit ions or confined ions ejected by some instability) depends heavily on the edge neutral density and all plasma profiles into the edge region. Regular measurements of edge profiles should be made or at least carried out during concerted campaigns. These profiles should extend to the wall beyond the usual $\rho = 1$ limit.

Very limited experimental run time required the use of conservative experimental methods designed to maximize the possibility of obtaining usable signals. One of the sacrifices made was the regular ramping of plasma current to assure that the first-orbits passed through the views. In future experiments, fixed plasma currents should provide a much-needed increase in signal levels.

7.2.3 Fast-Ion Instability Losses

Perhaps the most promising application of passive FIDA light and P-FIDAsim is the quantification of fast-ion losses from instabilities. The methods discussed in Section 6.2 could be taken to increasing levels of complexity and accuracy.

The first-order method already mentioned would be to output line-averaged fast-ion densities relative to experimentally-measured and simulation-quantified first-orbit densities. The issue here is the line-integrating nature of the signals and the linear
proportionality to neutral density. For example, a burst of fast-ions with a density $n_{fi}$ in a region along a LOS with a neutral density of $n_n$ would produce the same integrated signal as another burst with density $n_{fi}/2$ in a region with neutral density of $2n_n$. This makes no difference when using line-averaged values as in this case fast-ion density, neutral density, and emissivity are all considered uniform along the LOS. This method may give an accurate line-averaged fast-ion loss density, which will help in determining overall particle loss numbers. This, as a function of multiple chords, does give some spatial dependence, however, it will not give detailed spatial distributions and local values. For toroidally symmetric modes, such as the sawtooth, added spatial dependence is not necessary as is shown in Section 6.2.

The ideal implementation of these methods would be to have two or more intersecting sets of views to create tomographic reconstructions of both first-orbit light and instability-induced light. This would remove the ambiguity of line integration and allow first-orbit light to everywhere be compared with instability-loss light. The final result would be a 2D tomographic reconstruction of the fast-ion loss density.

The feasibility of this method is tested using sawtooth instabilities, which have the advantage of being small enough to allow for the concurrent measurement of first-orbit light. Stronger loss mechanisms such as ELMs may obscure the signals intended to measure the first-orbit light. Perhaps lower intensity or less frequent ELMs could still be worked around by careful time-slice selection. More options open up by working across multiple shots: for example, determining the first-orbit density in one shot and finding the instability loss levels in the next where the profiles are found to be or expected to be comparable.
7.2.4 Large Ion-Orbit Devices

A brief note is perhaps justified on the possibly unique opportunities available in applying these techniques to large ion-orbit devices such as MAST, NSTX, and Tri Alpha Energy’s C-2 field-reversed configuration (FRC)[45]. In principle, the same measurement and simulation of fast-ion edge light can be made on these devices. However, unlike the situation in a tokamak, a spherical tokamak and an FRC both have large ion orbits. This means there is a much larger fraction of ions that traverse the edge region and possibly charge exchange there to produce edge light. In this case, perhaps not only first-orbit and instability-induced light will be observed using a passive FIDA system, but also light that more heavily represents the confined fast-ion population. This may simply contribute to the background signal when looking at first-orbit or instability losses, or it may be an alternative method to investigate the outer-most region of the confined ion population.
Bibliography


Appendices

A P-FIDAsim Workflow

The passive FIDA simulation is located on the DIII-D server at /u/boltena/_NATHAN/PFIDASIM. The following workflow discussion will use this as the root directory.

The simulation has three main inputs: 1. A csv file (/DATA/exp_and_sim_configs.csv) 2. The plasma profiles extrapolated to the wall and 3. An IDL input file created by passive_inputs.pro.

All simulation runs are identified and referred to by a unique integer (normally referred to as fasti) which is generated and stored in exp_and_sim_configs.csv. The csv file allows for easy storage and manipulation of input data without the formatting required to put the data in IDL. The csv file also contains the shot number, start and end times, source beam, corrupting beam, which chords to use, what time to use for the equilibrium and profiles, and more. This file not only contains much needed data to run the simulation, but also has many open fields that are used to make comments and track experimental runs and simulations. Any new field can be added as long as the existing fields remain for simulation use.

The next set of inputs is the profiles. The profiles are extrapolated into the edge
region using /TOOLS/profiles_editor.pro. Having saved the raw profiles in /DATA/PROFILES, entering the desired fasti into profiles_editor will bring up the profiles and extrapolate them at the exponential rate chosen and save the processed profile data. The normalized neutral density is calculated separately by using /NEUTRAL_DENSITY/neutral2d.pro followed by /NEUTRAL_DENSITY/regularize_nn.pro. In the future, these codes should be combined and run automatically from the main simulation code.

The final set of inputs comes from passive_inputs.pro. This file defines directories for inputs and outputs as well as file names. The number of simulation ions is chosen, as are several atomic physics settings and orbit settings, and some booleans. All the inputs are saved as a structure.

The main simulation (passive_main.pro) is then run by calling it with the name of the file created by passive_inputs.pro. By default, if any portion of passive_main has already run and has the same inputs for this run as it had for the saved run, the previous run will be restored. If a single input has changed or any of the keywords are selected to run a new module, then a new run will be initiated. Passive_main then runs all the modules discussed in Section 4.1 (except for the normalized neutral density, as discussed, and some of the optional post-processing codes).

Experimental and simulated spectra can be compared by using /u/boltena/ANALYSIS/plot_exp_and_sim_spectra2.pro. This code applies the instrumental broadening function (created by /TOOLS/construct_kernel2.pro) and the instrumental response function (created by /TOOLS/instru_func.pro).